NBS MONOGRAPH 25 — SECTION 2

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# Standard X-ray Diffraction Powder Patterns



U.S. DEPARTMENT OF COMMERCE NATIONAL BUREAU OF STANDARDS

# THE NATIONAL BUREAU OF STANDARDS

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NATIONAL BUREAU OF STANDARDS . A. V. Astin, Director

# Standard X-ray Diffraction Powder Patterns

Howard E. Swanson, M. C. Morris, Roger P. Stinchfield, and Eloise H. Evans



National Bureau of Standards Monograph 25 — Section 2

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#### Standard X-ray Diffraction Powder Patterns

The ten previous volumes in this series are available from the Superintendent of Documents, U.S. Government Printing Office, Washington 25, D.C., as follows:

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# Errata

Circular 539
Vol. 8, Page 3, the hkl 314 should be 202.

Page 71, space group R3 should be R3m (No. 160).
Vol. 10, Page 32, the hkl 186 should be deleted.

Page 51, the hkl 201 should be 004.

Page 52, space group P2<sub>1</sub>/n is correct as originally printed.

Monograph 25 Sec. 1, Page 17, the radiation indicated in the table heading should be Co not Cu. Page 37, under  $NBS\ sample$ , chalcopurite should be chalcopyrite.

# STANDARD X-RAY DIFFRACTION POWDER PATTERNS

Section 2—Data for 37 Substances

Howard E. Swanson, Marlene Cook Morris, 1 Roger P. Stinchfield, and Eloise H. Evans 1

Standard X-ray diffraction powder patterns are presented for the following thirty-seven substances: Al (PO<sub>3</sub>)<sub>3</sub>, SbF<sub>3</sub>\*, Ba<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>\*, Ba(ClO<sub>4</sub>)<sub>2</sub>·3H<sub>2</sub>O, Cd(CN)<sub>2</sub>\*, CdWO<sub>4</sub>, Cs<sub>2</sub>OsBr<sub>6</sub>\*, Cs<sub>2</sub>OsCl<sub>6</sub>\*, α-CrPO<sub>4</sub>, Co[Hg(CNS)<sub>4</sub>]\*, β-CoSO<sub>4</sub>, Dy<sub>3</sub>Ga<sub>2</sub> (GaO<sub>4</sub>)<sub>3</sub>\*, ErMnO<sub>3</sub>\*, Eu<sub>3</sub>Ga<sub>2</sub> (GaO<sub>4</sub>)<sub>3</sub>\*, Gd<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub>\*, Li<sub>3</sub>AsO<sub>4</sub>\*, Li<sub>3</sub>P<sub>3</sub>O<sub>9</sub>·3H<sub>2</sub>O\*, Li<sub>2</sub>WO<sub>4</sub>·½H<sub>2</sub>O\*, Lu<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub>\*, LuMnO<sub>3</sub>\*, MnWO<sub>4</sub> (huebnerite), HgF<sub>2</sub>\*, NiSO<sub>4</sub>, NiWO<sub>4</sub>\*, K<sub>2</sub>ReCl<sub>6</sub>, K<sub>2</sub>RuCl<sub>5</sub>NO\*, RbClO<sub>4</sub>\*, RbIO<sub>4</sub>\*, Ag<sub>2</sub>SeO<sub>4</sub>\*, NaCNO\*, Na<sub>2</sub>WO<sub>4</sub>·2H<sub>2</sub>O, β-Na<sub>4</sub>P<sub>4</sub>O<sub>12</sub>·4H<sub>2</sub>O, Sr<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>\*, Tl<sub>3</sub>AsO<sub>4</sub>\*, TlClO<sub>4</sub>\*, YAsO<sub>4</sub>, ZnWO<sub>4</sub>\*. Eleven are to replace patterns already given in the X-ray Powder Data File issued by the American Society for Testing and Materials, and twenty-six patterns indicated by asterisks are for substances not previously included. The X-ray Powder Data File is a compilation of diffraction patterns from many sources and is used for the identification of unknown crystalline materials by matching spacing and intensity measurements. The patterns were made with a Geiger counter X-ray diffractometer, using samples of high purity. When possible, the d-values were assigned Miller indices determined by comparison with calculated interplanar spacings and from space group extinctions. The densities Standard X-ray diffraction powder patterns are presented for the following thirty-seven with calculated interplanar spacings and from space group extinctions. The densities and lattice constants were calculated, and the refractive indices were measured whenever possible.

# INTRODUCTION

The National Bureau of Standards in its program<sup>2</sup> for the revision and evaluation of published X-ray data for the X-ray Powder Data File presents data in this report for 37 compounds. This paper is the twelfth of a series of "Standard X-ray Diffraction Patterns." The designation "Circular 539" used previously has been discontinued in favor of the new series, "Monograph 25." This is the second section of the new series Monograph 25. Included are patterns recommended to replace data on 11 cards now present in the file. The patterns for 26 compounds not

included in the file have been added. These compounds are: antimony(III) fluoride, barium arsenate, cadmium cyanide, cesium bromoosmate(IV), cesium chloroosmate(IV), cobalt mercury thiocyanate, dysprosium gallium oxide 3:5, erbium manganite, europium gallium oxide 3:5, gadolinium gallium oxide 3:5, lithium arsenate, lithium trimetaphosphate trihydrate, lithium tungstate hemihydrate, lutetium gallium oxide 3:5, lutetium manganite, mercury(II) fluoride, nickel tungstate, potassium nitroso chlororhenate, rubidium perchlorate, rubidium periodate, silver selenate, sodium cyanate, strontium arsenate, thallium arsenate, thallium(II) perchlorate, and zinc tungstate.

The experimental procedure and general plan of these reports have not changed greatly from previous volumes of the NBS Circular (see ref. 3). However, the basic technique is discussed, in this section, with minor changes that affect this volume's data.

<sup>&</sup>lt;sup>1</sup> Research Associate at the National Bureau of Standards sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods.

<sup>2</sup> This project is sponsored by the Joint Committee on Chemical Analysis by Powder Diffraction Methods. This committee is composed of members from the American Society for Testing and Materials, the American Crystallographic Association, and the British Institute of Physics. Financial support is also provided by the National Bureau of Standards.

<sup>2</sup> Other volumes were published as follows: Vol. 1 and Vol. 2, June 1953; Vol. 3, June 1954; Vol. 4, March 1955; Vol. 5, Octoher 1955; Vol. 6, September 1956; Vol. 7, September 1957; Vol. 8, April 1959; Vol. 9, February 1960; Vol. 10, September 1960; and Monograph 25—Section 1, March 1962.

Powder Data cards. Each section of this Monograph contains a table listing the Powder Data File card numbers, the three strongest lines, the radiation used, and the literature references for each card. Cards listed through the 1961 index to the Powder Data File [1] <sup>4</sup> are included in the table.

Additional published patterns. Literature references for patterns that have not been published

as Powder Data cards are listed.

NBS sample. Many of the samples used to make NBS patterns were special preparations of high purity obtained from a variety of sources or prepared in small quantities in our laboratory by J. de Groot. Unless otherwise noted, the spectrographic analyses were done at NBS after recrystallization or heat treatment of the sample. The limit of detection for the alkali elements was 0.05 percent for the spectrographic analysis. A phase purity check was made on the nonopaque materials during the refractive index determination. Another check of phase purity was usually provided by the X-ray pattern itself, when it was indexed by comparison with theoretical d-values. Treating the sample by appropriate annealing, recrystallization, or heating in hydrothermal bombs improved the quality of most of the pat-The refractive index measurements were made by grain-immersion methods in white light

using oils standardized in sodium light.

X-ray techniques. At least three patterns for intensity measurements were prepared to check reproducibility. Samples that gave satisfactory intensity patterns usually had an average particlesize smaller than  $10\mu$ , as discussed by Alexander, Klug, and Kummer [2]. A special cell with one open end was used for making intensity measurements. The sample was prepared by clamping a flat piece of glass temporarily over the surface of this holder, and while it was held in a vertical position, the sample was drifted in from the open end. The glass was then carefully removed so that the surface of the sample could be exposed to the X-ray beam. To powders that did not flow readily or were prone to orient excessively, approximately 50-volume percent of finely ground silica-gel was added as a diluent. The intensities of the diffraction lines were measured as peak heights above background and were expressed in percentages of the intensity of the strongest line. Additional patterns were obtained for d-value measurements. Specimens for these patterns were prepared by packing into a shallow holder a sample containing approximately 5-wt percent tungsten powder that served as an internal standard. When tungsten lines were found to

interfere, 25 percent silver was used in place of tungsten. The lattice constants used were 3.1648 A for tungsten and 4.0861 A for silver at 25 °C, as determined by Jette and Foote [3]. All of the NBS patterns, unless otherwise noted, are made at 25° C, using either filtered copper or cobalt radiation ( $K_{\alpha 1}$ ), having the wavelengths 1.5405 A, and 1.7889 A, respectively.

Structural data. For cubic materials a value for the lattice constant was calculated for each d-value. However, the constant reported is that obtained by averaging the last five lines because of the greater accuracy of measurement in the large-angle region of the pattern. The unit cell values for each noncubic substance were determined by means of a least-squares calculation made on the IBM 7090, using those d-values for which only one set of Miller indices could be assigned. The number of significant figures reported for d-values in the NBS pattern is limited by the quality of each sample as indicated by residuals obtained from least squares refinement.

Published unit cell data in kX units were converted to angstrom units as recommended in

1946 [4] using the factor 1.00202.

The space groups are listed with both the Schoenflies and short Hermann-Mauguin symbols as well as the space group numbers given in the International Tables for X-ray Crystallography [5].

Orthorhombic cell dimensions are presented according to the Dana convention [6] b > a > c.

The densities calculated from the NBS lattice constants are expressed in grams per cubic centimeter and are based upon atomic weights reported by E. Wichers [7] in 1956 and the Avogadro number  $(6.0240 \times 10^{23})$  reported by Straumanis [8] in 1954.

# References

[1] Index to the X-ray Powder Data File, American Society for Testing and Materials, Philadelphia, Pa. (1961).

[2] L. Alexander, H. P. Klug, and E. Kummer, Statistical factors affecting the intensity of X-rays diffracted by crystalline powders, J. Appl. Phys. 19, No. 8, 742– 753 (1948).

[3] E. R. Jette and F. Foote, Precision determination of lattice constants, J. Chem. Phys. 3, 605-616 (1935).

[4] Anonymous, The conversion factor for kX units to angstrom units, J. Sci. Inst. 24, 27 (1947).

[5] International Tables for X-ray Crystallography, 1, 1952.

[6] Dana's System of Mineralogy, 1, 6 (1944).

[7] E. Wichers, Report of the Committee on Atomic Weights of the American Chemical Society, J. Am. Chem. Soc. 78, 3235 (1956).

[8] M. E. Straumanis, Remarks concerning the absolute value of Avogadro's number, Phys. Rev. 95, 566

(1954).

 $<sup>^{4}</sup>$  Figures in brackets indicate the literature references at the  ${\bf end}$  of each section of this paper.

# Aluminum Metaphosphate, Al(PO<sub>3</sub>)<sub>3</sub> (cubic)

# Powder Data cards

Card number	Index lines	Radiation	Source
2-0246	4. 38 3. 70 3. 41	Molyb- denum	Hendricks and Wyckoff [1] 1927.

Additional published patterns. None.

NBS sample. The sample of aluminum metaphosphate was made at NBS by adding fine  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> powder to hot HPO<sub>3</sub>. The sample was then heated to fume off the excess acid. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of silicon and platinum; and 0.001 to 0.01 percent each of barium, iron, magnesium, nickel, lead, and antimony.

The sample is colorless. The index of refrac-

tion is 1.545.

The d-values of the three strongest lines are:

4.34, 3.43, and 3.67 A.

Structural data. Hendricks and Wyckoff [1] determined in 1927 that aluminum metaphosphate has the space group  $T_d^6$ — $\overline{14}3d$  (No. 220) and  $16[Al(PO_3)_3]$  per unit cell:

The lattice constant reported by Hendricks and Wyckoff has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

1927 Hendricks and Wyckoff [1] 13.60 National Bureau of Standards_ 25
--

The density of aluminum metaphosphate calculated from the NBS lattice constant is 2.709 g/cm<sup>3</sup> at 25 °C.

#### Reference

1] S. B. Hendricks and R. W. G. Wyckoff, The space group of aluminum metaphosphate, Am. J. Sci. 213 No. 13, 491-496 (1927).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	I	a
211 220 310 321 400	A 5. 61 4. 85 4. 34 3. 67 3. 432	25 17 100 57 62	A 13. 73 13. 72 13. 72 13. 72 13. 73
420	3. 070	30	13. 73
332	2. 927	46	13. 73
422	2. 801	5	13. 72
510	2. 692	28	13. 73
521	2. 507	13	13. 73
530	2. 354	22	13. 73
611	2. 227	17	13. 73
620	2. 171	11	13. 73
541	2. 118	5	13. 73
631	2. 024	2	13. 73
$\begin{array}{c} 444 \\ 710 \\ 640 \\ 721 \\ 642 \end{array}$	1. 981	9	13. 72
	1. 941	7	13. 72
	1. 903	6	13. 72
	1. 869	18	13. 73
	1. 835	2	13. 73
732	1. 743	13 $2$ $14$ $6$ $12$	13. 73
811	1. 6900		13. 73
820	1. 6648		13. 728
653	1. 6412		13. 730
822	1. 6179		13. 728
831	1. 5963	18	13. 732
752	1. 5549	2	13. 732
840	1. 5349	1	13. 729
842	1. 4986	11	13. 730
921	1. 4803	10	13. 728
930	1. 4473	11	13. 730
932	1. 4161	7	13. 730
844	1. 4013	3	13. 730
941	1. 3870	5	13. 731
10·0·0	1. 3730	1	13. 730
$10 \cdot 1 \cdot 1$ $10 \cdot 2 \cdot 0$ $950$ $10 \cdot 3 \cdot 1$ $871$	1. 3594	2	13. 729
	1. 3462	5	13. 729
	1. 3333	2	13. 727
	1. 3092	7	13. 731
	1. 2860	5	13. 731
$\begin{array}{c} 10.4.0 \\ 10.3.3 \\ 10.4.2 \\ 11.1.0 \\ 11.2.1 \end{array}$	1. 2748	2	13. 730
	1. 2641	4	13. 732
	1. 2532	1	13. 728
	1. 2433	7	13. 733
	1. 2231	8	13. 729
880	1. 2135	<1	13. 729
11·3·0	1. 2042	3	13. 730
11·3·2	1. 1862	6	13. 731
10·6·0	1. 1772	1	13. 728
11·4·1	1. 1688	3	13. 730

# Aluminum Metaphosphate, Al(PO<sub>3</sub>)<sub>3</sub> (cubic)—Continued

1			
hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	I	a
10· 6·2 965 12· 1·1 12· 2·0 11· 5·2	A 1. 1605 1. 1522 1. 1364 1. 1287 1. 1212	5 2 8 <1 2	A 13. 731 13. 730 13. 731 13. 731 13. 731
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	1. 1137	2	13, 731
	1. 1064	1	13, 730
	1. 0924	1	13, 731
	1. 0722	1	13, 731
	1. 0657	1	13, 731
10· 8·2	1. 0594		13. 731
13· 1·0	1. 0529		13. 729
13· 2·1	1. 0409		13. 730
12· 4·4	1. 0348		13. 728
13· 3·0	1. 0291		13. 730
13. 3.2	1. 0177	$     \begin{array}{c}                                     $	13. 730
12. 6.2	1. 0121		13. 729
13. 4.1	1. 0067		13. 730
888	0. 9910		13. 732
13. 5.0	. 9857		13. 729
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	. 9759	1	13. 732
	. 9709	2	13. 731
	. 9661	1	13. 731
	. 9567	3	13. 731
	. 9521	<1	13. 731
13· 5·4	. 9475	3	13. 731
14· 3·3	. 9385	1	13. 729
14· 4·2	. 9343	1	13. 731
13· 7·0	. 9299	3	13. 730
14· 5·1	. 9215	3	13. 730

hkl	1962 National Burea of Standards Cu, 1.5405 A at 25 ° Internal standard, tungsten, $a=3.1648$		°C
	d	I	а
12. 8.4 15. 2.1 15. 3.0 14. 6.2 15. 3.2	A . 9173 . 9051 . 8975 . 8937 . 8900	<1 3 2 2 <1	A 13. 729 13. 727 13. 729 13. 729 13. 730
15· 4·1	. 8826	3	13. 730
12·10·0	. 8789	2	13. 729
14· 7·1	. 8754	2	13. 730
14· 6·4	. 8718	1	13. 729
15· 5·0	. 8683	2	13. 729
15. 5.2 16. 1.1 16. 2.0 15. 6.1 16. 3.1	. 8615 . 8547 . 8513 . 8482 . 8418	3 3 3 5	13. 730 13. 729 13. 727 13. 729 13. 729
15· 6·3	. 8356	3	13. 730
16· 4·0	. 8325	1	13. 730
16· 3·3	. 8295	4	13. 731
15· 7·2	. 8235	4	13. 730
16· 5·1	. 8176	3	13. 730
15· 6·5	. 8118	2	13. 729
17· 1·0	. 8062	3	13. 729
17· 2·1	. 8007	1	13. 729
16· 6·2	. 7980	2	13. 729
17· 3·0	. 7953	1	13. 729
$ \begin{array}{c cccc} 17 \cdot & 3 \cdot 2 \\ 17 \cdot & 4 \cdot 1 \\ 16 \cdot & 6 \cdot 4 \end{array} $	. 7900	1	13. 729
	. 7849	5	13. 730
	. 7823	3	13. 729

# Antimony(III) Fluoride, SbF<sub>3</sub> (orthorhombic)

Powder Data cards. None. Data on ASTM card 1-0523 probably represents oxyfluoride produced when antimony fluoride is exposed in air

Additional published patterns. None.

NBS sample. The sample of antimony fluoride was obtained from City Chemical Company, New York, N.Y. The material was sublimed at NBS and then mixed with silicone grease to protect it from oxidation in the atmosphere. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum iron, magnesium, and silicon.

The sample was colorless and optically negative with the indices of refraction  $N_{\alpha}=1.587$ ,  $N_{\beta}=$ 

1.615, and  $N_{\gamma} = 1.629$ .  $2V = \sim 65^{\circ}$ .

The d-values of the three strongest lines are: 3.621, 3.728, and 1.810 A.

Structural data. Byström and Westgren [1] in 1943 determined that antimony(III) fluoride is orthorhombic with the space group  $C_2^{16}$ —Ama2 (No. 40) and  $4(SbF_3)$  per unit cell. The lattice constants of Byström and Westgren have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	С
1943 1962	Byström and Westgren. National Bureau of Standards.	$egin{array}{c} A \\ 7.26 \\ 7.241 \end{array}$	$egin{array}{c} A \\ 7.51 \\ 7.456 \end{array}$	A 4. 96 4. 940 at 25 °C

# Antimony (III) Fluoride, SbF<sub>3</sub> (orthorhombic)—Continued

The density of antimony(III) fluoride calculated from the NBS lattice constants is 4.451 g/cm³ at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard tungsten, a=3.1648 A	
	d	I
	4	
020 200 111 120 211	A 3. 728 3. 621 3. 580 3. 317 2. 718	53 100 16 3
211	2. 718	<1
220 002 031 131 311	2. 597 2. 472 2. 221 2. 123 2. 083	${<_{1}^{4}\atop {6}\atop {6}\atop {5}}$
022 202 320 122 231	2. 059 2. 040 2. 028 1. 981 1. 892	1 1 2 1 2
$040 \\ 400 \\ 140 \\ 222 \\ 240, 411$	1. 864 1. 810 1. 805 1. 790 1. 656	$   \begin{array}{c}     8 \\     21 \\     13 \\     2 \\     1   \end{array} $
331 420 113 322 042	1. 633 1. 6284 1. 5697 1. 5668 1. 4875	$\begin{array}{c} 2 \\ 2 \\ < 1 \\ < 1 \end{array}$
340 402 142 051 431	1. 4756 1. 4605 1. 4580 1. 4279 1. 4028	$     \begin{array}{c}       1 \\       1 \\       1 \\       2 \\       1     \end{array} $

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard tungsten, a=3.1648 A	
	d	I
151 242 511 422 520	$\begin{matrix} A \\ 1.\ 4003 \\ 1.\ 3760 \\ 1.\ 3661 \\ 1.\ 3594 \\ 1.\ 3503 \end{matrix}$	$\begin{array}{c} 2 \\ < 1 \\ 3 \\ < 1 \\ < 1 \end{array}$
133 313 251 440 233	1. 3486 1. 3379 1. 3282 1. 2986 1. 2834	$egin{array}{c} < 1 \\ < 1 \\ < 1 \\ < 1 \end{array}$
342 004 351 160 531	1. 2667 1. 2348 1. 2286 1. 2249 1. 2130	<1 <1 <1 1 <1
600 333 522 024 204	1. 2069 1. 1930 1. 1841 1. 1724 1. 1695	$\begin{array}{c c} 4\\ <1\\ <1\\ <1\\ \end{array}$
611 124 620 540 451	1. 1584 1. 1566 1. 1484 1. 1433 1. 1208	$\begin{array}{c c} <1\\ <1\\ 3\\ <1\\ <1\end{array}$
$\begin{array}{c} 224 \\ 053,  360 \\ 162 \\ 602 \\ 513 \end{array}$	1. 1155 1. 1049 1. 0971 1. 0844 1. 0760	<1 <1 <1 <1 <1
631 253 071, 622 542	1. 0605 1. 0573 1. 0413 1. 0376	$\begin{array}{c} <1\\<1\\1\\<1\end{array}$

# Reference

[1] A. Byström and A. Westgren, X-ray analysis of antimony trifluoride, Arkiv. Kemi, Mineral. Geol. 17B, No. 2, 1–8 (1943).

# Barium Arsenate, Ba<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub> (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of barium arsenate was prepared at NBS by reacting solutions of barium chloride and arsenic(V) acid. The precipitate was washed several times, dissolved in nitric acid, reprecipitated by addition of ammonia, and heated at 1,000 °C for 1 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium and strontium; and 0.001 to 0.01 percent each of aluminum, chromium, lead, megnesium, and silicon.

The sample was colorless and too fine-grained to allow determination of the indices of refraction.

The d-values of the three strongest lines are: 3.24, 2.888, and 2.1532 A.

hkl (hex.)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A	
	d	I
003 101 104 015 110	A 7. 08 4. 88 3. 64 3. 24 2. 888	<1 4 7 100 89
$021 \\ 202 \\ 009 \\ 024 \\ 116$	2. 482 2. 433 2. 356 2. 260 2. 2360	1 6 7 7 1
$205 \\ 1 \cdot 0 \cdot 10 \\ 211 \\ 119 \\ 214$	2. 1532 1. 9521 1. 8819 1. 8246 1. 7797	43 26 2 8 2
$\begin{array}{c} 125 \\ 300 \\ 0 \cdot 2 \cdot 10 \\ 2 \cdot 0 \cdot 11 \\ 0 \cdot 1 \cdot 14 \end{array}$	1. 7262 1. 6667 1. 6168 1. 5258 1. 4491	$\begin{array}{c c} 30 \\ 16 \\ 11 \\ < 1 \\ 4 \end{array}$
$220$ $2 \cdot 1 \cdot 10$ $309$ $134$ $315$	1. 4433 1. 4108 1. 3606 1. 3421 1. 3180	$\begin{array}{c c} 13 \\ 18 \\ 2 \\ < 1 \\ 12 \end{array}$
2.0.14 $1.1.15$ $229$ $404$ $045$	1. 2957 1. 2696 1. 2306 1. 2166 1. 1990	$\begin{bmatrix} 2\\11\\3\\<1\\5 \end{bmatrix}$
1.2.14 $0.2.16$ $1.3.10$ $235$ $410$	1. 1816 1. 1705 1. 1605 1. 1073 1. 0911	$begin{pmatrix} 3 \\ <1 \\ 9 \\ 6 \\ 6 \\ 6 \\ \end{bmatrix}$

Structural data. Durif [1] in 1959 determined that barium arsenate is isostructural with barium phosphate, with the space group D<sub>3d</sub><sup>5</sup>-R<sub>3</sub>m (No. 166) and 1[Ba<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>] per rhombohedral unit cell or 3[Ba<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub>] per hexagonal unit cell.

Lattice constants

		a	c
1959 1962	Durif [1] National Bureau of Standards.	A 5. 753 5. 774	A 21. 18 21. 204 at 25 °C

hkl (hex.)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A		
	d	I	
$3.0.15,413 \\ 4.0.10 \\ 0.1.20 \\ 3.1.14 \\ 2.2.15,0.0.21 \\ 3.2.10$	A 1. 0780 1. 0767 1. 0370 1. 0228 1. 0096 1. 0090	10 5 2 1 6	
$ \begin{array}{c} 419 \\ 2 \cdot 0 \cdot 20 \\ 505 \\ 0 \cdot 4 \cdot 14 \end{array} $	. 9901 . 9761 . 9736 . 9638	$\begin{bmatrix} 2\\1\\2\\2 \end{bmatrix}$	
$ \begin{array}{r} 330,3 \cdot 0 \cdot 18 \\ 2 \cdot 1 \cdot 19 \\ 422 \\ 244 \\ 1 \cdot 2 \cdot 20 \end{array} $	. 9621 . 9611 . 9410 . 9305 . 9246	$\begin{pmatrix} 3 \\ 4 \\ < 1 \\ 1 \\ 4 \end{pmatrix}$	
$\begin{array}{r} 425 \\ 2 \cdot 3 \cdot 14 \\ 0 \cdot 5 \cdot 10 \\ 339 \\ 0 \cdot 0 \cdot 24 \end{array}$	. 9224 . 9144 . 9045 . 8909 . 8836	$egin{array}{c} 7 \\ 3 \\ 2 \\ 1 \\ < 1 \end{array}$	
$\begin{array}{c} 155 \\ 1 \cdot 3 \cdot 19 \\ 4 \cdot 1 \cdot 15, 3 \cdot 0 \cdot 21 \\ 3 \cdot 3 \cdot 12, 1 \cdot 1 \cdot 24 \\ 3 \cdot 1 \cdot 20 \end{array}$	. 8786 . 8695 . 8636 . 8449 . 8424	4 3 10 3 3	
$\begin{array}{c} 1.0.25 \\ 5.0.14 \\ 600 \\ 5.1.10 \\ 0.4.20 \end{array}$	. 8362 . 8344 . 8334 . 8269 . 8086	1 2 2 4 1	
$\begin{array}{c} 345 \\ 0.1.26 \\ 0.2.25 \\ 520 \\ 3.2.19 \end{array}$	. 8070 . 8050 . 8032 . 8007 . 8000	$\begin{array}{c}4\\3\\1\\6\\3\end{array}$	
$\begin{array}{c} 523,3\cdot 3\cdot 15 \\ 609 \\ 3\cdot 0\cdot 24 \end{array}$	. 7955 . 7857 . 7807	$egin{array}{c} 4 \\ 1 \\ 3 \end{array}$	

The density of barium arsenate calculated from the NBS lattice constants is 5.612 g/cm<sup>3</sup> at 25 °C.

# Reference

[1] A. Durif, Structure cristalline des orthovanadates etorthoarseniates de baryum et de strontium, Acta-Cryst. 12, 420–421 (1959).

# Barium Perchlorate Trihydrate, Ba(ClO<sub>4</sub>)<sub>2</sub>·3H<sub>2</sub>O (hexagonal)

#### Powder Data cards

Card number	Index	Radiation	Source
1-0931	2. 90 3. 65 2. 14	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

# Additional published patterns. None.

NBS sample. The sample of barium perchlorate trihydrate was prepared at NBS by the reaction of solutions of barium carbonate and perchloric acid. The sample was purified by recrystallization. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, calcium, chromium, iron, magnesium, and sodium.

The sample was colorless and optically negative with the refractive indices  $N_0=1.533$  and  $N_0=1.533$ 

The d-values of the three strongest lines are:

3.646, 2.912, and 4.84 A.

Structural data. West [2] in 1934 determined that barium perchlorate trihydrate is hexagonal with the space group  $C_6^6$ — $P6_3$  (No. 173) or  $C_{6h}^2$ — $P6_3/m$  (No. 176) and  $2[Ba(ClO_4)_2 \cdot 3H_2O]$  per unit cell. The unit cell measurements of West [2] have been converted from kX to angstrom units for comparison with the NBS values.

#### Lattice constants

		a	С
1934 1960	West [2] Mani and Ramaseshan	A 7. 295 7. 278	A 9. 659 9. 64
1962	[3]. National Bureau of Standards.	7. 294	9. 674 at 25 °C.

The density of barium perchlorate trihydrate calculated from the NBS lattice constants is 2.907 g/cm³ at 25 °C.

#### References

J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-512 (1938).
 C. D. West, Crystal structures of some hydrated compounds, Z. Krist. 88A, 198-204 (1934).
 N. V. Mani and S. Ramaseshan, The crystal structure of barium perchlorate trihydrate Ba(ClO<sub>4</sub>)<sub>2</sub>·3H<sub>2</sub>O and the crystal coordination of Ba<sup>++</sup> ion. Z. Krist.

and the crystal coordination of Ba++ ion, Z. Krist. **114,** 200–214 (1960).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	I
100 002 102 110 200	A 6. 32 4. 84 3. 839 3. 646 3. 158	34 36 15 100 3
112 103 202 004 210	2. 912 2. 872 2. 644 2. 422 2. 389	73 14 13 8 14
211 104, 203 212 300 301	2. 317 2. 257 2. 142 2. 106 2. 057	$\begin{array}{c} 6 \\ 21 \\ 25 \\ 18 \\ 2 \end{array}$
114 302 204, 213 220 310	2. 015 1. 9309 1. 9197 1. 8250 1. 7524	9 19 6 5
222 214 205 312 304, 223	1. 7069 1. 6995 1. 6485 1. 6472 1. 5880	5 2 4 2 7
400 106 401 313 402	1, 5790 1, 5618 1, 5582 1, 5388 1, 5009	$\begin{bmatrix} 5 \\ 2 \\ 1 \\ < 1 \\ 6 \end{bmatrix}$
116 224 320 206 314	1. 4744 1. 4564 1. 4493 1. 4363 1. 4196	9 3 2 5 3
322 410 216 412 404, 323	1. 3875 1. 3780 1. 3364 1. 3253 1. 3222	5 9 5 7 5
306 500 324 502 330	1. 2801 1. 2629 1. 2432 1. 2221 1. 2157	$<_{1}^{2}$ $<_{1}^{3}$ $<_{1}^{3}$
226 414 316 332	1. 2080 1. 1975 1. 1866 1. 1787	1 2 2 3

# Cadmium Cyanide, Cd(CN)<sub>2</sub> (cubic)

Powder Data cards. None.

Additional published pattern. Shugam and

Zhdanov [1] 1945.

NBS sample. The sample of cadmium cyanide was prepared at NBS from solutions of cadmium chloride and sodium cyanide. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent sodium; 0.01 to 0.1 percent silicon; and 0.001 to 0.01 percent each of aluminum, barium, calcium, iron, nickel, and titanium.

The color of the sample was white. The index of

refraction is 1.443.

The *d*-values of the three strongest lines are:

4.458, 2.575, and 2.229 A. Structural data. Shugam and Zhdanov [1] in 1945 determined that cadmium cyanide has the cuprous oxide structure, the space group T<sub>d</sub> -- P43m (No. 215), and 2[Cd(CN)<sub>2</sub>] per unit cell. The lattice constant reported by Shugam and Zhdanov has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

		A
1945 1962	Shugam and Zhdanov [1] National Bureau of Standards_	6. 33 6.3050 at 25 °C

The density of cadmium cyanide calculated from the NBS lattice constant is 2.178 g/cm<sup>3</sup> at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	I	a
	A		A
110	4, 458	100	6. 305
111	3. 640	7	6. 304
200	3. 153	6	6. 306
211	2. 575	32	6. 307
220	2. 229	13	6. 305
310	1. 9935	8	6. 304
222	1. 8198	2	6. 304
321	1. 6851	6	6. 3050
411	1. 4860	3	6. 3046
420	1. 4099	8 2 6 3 <1	6. 3052
332	1. 3442	$<_1$	6. 3049
510	1. 2366	1	6. 3054
Average	value of last five	· lines	6. 3050

## Reference

[1] E. A. Shugam and G. S. Zhdanov, The crystal structure of cadmium cyanide, Acta Physicochim. U. R. S. S. 20, 247-252 (1945).

# Cadmium Tungstate, CdWO<sub>4</sub> (monoclinic)

#### Powder Data cards

Card number	Index	Radiation	Source
1-0488	3. 80 3. 05 2. 53	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. Coing-Boyat

[2] 1961.

NBS sample. The sample of cadmium tungstate was prepared at NBS from solutions of cadmium chloride and sodium tungstate. The precipitate was washed several times and then heated to 800 °C for 10 min. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent sodium; and 0.001 to 0.01 percent silicon.

The color of the sample was pale yellow. The indices of refraction could not be determined because the sample was too fine-grained.

The d-values of the three strongest lines are:

3.077, 3.020, and 2.536 A.

Structural data. Coing-Boyat [2] in 1961 determined that cadmium tungstate is monoclinic with the most probable space group  $C_{2h}^5-P2_1/c$  (No. 14) and 2 (CdWO<sub>4</sub>) per unit cell and is probably isostructural with MgWO<sub>4</sub>. Sharp [3] in 1960 reported that the most probable space group for cadmium tungstate was C<sub>2h</sub>-P2<sub>1</sub>/b (No. 14); however, this space group did not completely satisfy our data.

# Cadmium Tungstate, CdWO4 (monoclinic)—Continued

hkt	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, $a=4.0861$ A	
	d	I
010 100 110 111 111	A 5. 87 5. 04 3. 818 3. 077 3. 020	7 12 43 100 87
$\begin{array}{c} 020 \\ 021,002 \\ 200 \\ \underline{210} \\ \overline{102} \end{array}$	2. 928 2. 536 2. 514 2. 311 2. 287	26 54 23 2 3
$ \begin{array}{c} 121 \\ \overline{1}12 \\ 112 \\ 030 \\ 022 \end{array} $	2. 253 2. 131 2. 092 1. 953 1. 916	7 5 8 2 18
$\begin{array}{c} 220 \\ 130 \\ \overline{2}02 \\ \overline{2}21 \\ 221 \end{array}$	1. 907 1. 820 1. 809 1. 797 1. 774	17 23 17 16 21
$ \begin{array}{r} 202 \\ \overline{1}31 \\ 131 \\ 212 \\ 310 \end{array} $	1. 762 1. 718 1. 708 1. 688 1. 611	13 4 2 <1 3
$ \begin{array}{r}                                     $	1. 557 1. 546 1. 543 1. 539 1. 535	15 14 12 10 13
$ \begin{array}{c c} 311 \\ 222 \\ \hline 132 \\ 132 \\ 040, 023 \end{array} $	1. 524 1. 510 1. 485 1. 472 1. 465	12 6 10 11 9

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, silver, $a=4.0861$ A	
	d	I
$egin{array}{c} \overline{1}23 \\ 041 \\ \overline{2}13 \\ \overline{3}12 \\ \overline{1}41 \\ \end{array}$	A 1. 414 1. 407 1. 379 1. 375 1. 357	$\begin{array}{c} 1 \\ 11 \\ 2 \\ 2 \\ 1 \end{array}$
141 213 312 232 232	1. 353 1. 350 1. 345 1. 327 1. 308	<1 <1 1 1 <1
$\begin{array}{c} 033,\overline{2}23\\ 330\\ 042\\ 400\\ 223\\ \end{array}$	1. 278 1. 272 1. 268 1. 257 1. 254	3 6 5 5 4
$\begin{bmatrix} \overline{3}31 \\ \overline{2}41 \\ 241 \\ \overline{1}14 \\ \overline{3}13 \end{bmatrix}$	1. 238 1. 2319 1. 2242 1. 2105 1. 1814	$egin{pmatrix} <1 & & & & & & & & & & & & & & & & & & $
$\begin{array}{c} 024 \\ 420 \\ 313 \\ \overline{3}32 \\ \overline{2}04 \end{array}$	1. 1638 1. 1549 1. 1522 1. 1458 1. 1435	2 3 5 6 1
$\begin{array}{c} 051 \\ \overline{421} \\ 332, 124 \\ 204 \\ \overline{323} \end{array}$	1. 1415 1. 1321 1. 1285 1. 1206 1. 1149	6 3 4 3 4
043	1. 1072	3

Lattice constants

	a	ь	c	β
vat [2] Bureau of Standards	A 5. 028 5. 026 5. 029	A 5. 868 5. 854 5. 859	A 5. 076 5. 074 5. 074	91. 45° 91. 48° 91. 47 at 25°C

# References

- J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by x-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-512 (1938).
   J. Coing-Boyat, Groupe d'espace du tungstate de cadmium, CdWO<sub>4</sub>, Acta Cryst. 14, 1100 (1961).
   W. E. Sharp, Lattice constants of CdWO<sub>4</sub>, Z. Krist. 114, 151-153 (1960).

The density of cadmium tungstate calculated from the NBS lattice constants is 8.003 g/cm³ at 25 °C.

# Cesium Bromoosmate (IV), Cs<sub>2</sub>OsBr<sub>6</sub> (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium bromoosmate was prepared at NBS by R. Johannesen from solutions of cesium bromide and bromoosmic acid. Spectrographic analysis showed the only major impurity to be 0.001 to 0.01 percent of sodium.

The color of the sample was very dark brown. The refractive index could not be determined because the sample was too fine-grained.

The *d*-values of the three strongest lines are:

2.665, 3.077, and 6.154 A.

Structural data. The structure of cesium bromoosmate has not been reported. However, because of the similarity of patterns, it is thought to be isostructural with ammonium bromoosmate having the space group O<sub>h</sub><sup>5</sup>—Fm3m (No. 225) with 4(Cs<sub>2</sub>OsBr<sub>6</sub>) per unit cell.

Lattice constant

$\begin{bmatrix} 1962 & \text{National Bureau of Standards.} \end{bmatrix}$ $\begin{bmatrix} A \\ 10.659 \text{ at} \\ 25 \text{ °C.} \end{bmatrix}$	]	1962	National Bureau of Standards_	
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The density of cesium bromoosmate calculated from the NBS lattice constant is 5.130 g/cm³ at 25 °C.

hkl	Cu, 1.	f Standards 5 °C ard, 48 A	
	d	I	a
111 200 220 311 222	A 6. 154 5. 239 3. 770 3. 214 3. 077	79 7 63 26 91	A 10. 659 10. 658 10. 663 10. 660 10. 659
400 $331$ $420$ $422$ $511$	2. 665 2. 4466 2. 3844 2. 1765 2. 0517	$100 \\ 5 \\ 4 \\ 21 \\ 18$	10. 660 10. 664 10. 663 10. 663 10. 661
440	1. 8844	61	10. 660
531	1. 8017	16	10. 659
600	1. 7762	3	10. 657
620	1. 6851	9	10. 658
533	1. 6252	5	10. 657
622 $444$ $711$ $640$ $642$	1. 6067	18	10. 658
	1. 5382	16	10. 657
	1. 4923	8	10. 657
	1. 4780	3	10. 658
	1. 4242	8	10. 658
731 800 822 751 622	1. 3875	4	10. 658
	1. 3321	5	10. 657
	1. 2560	3	10. 658
	1. 2307	3	10. 658
	1, 2225	5	10. 658
840	1. 1920	12	10. 662
911	1. 1700	3	10. 659
664	1. 1361	3	10. 658
931	1. 1172	4	10. 657
844	1. 0879	7	10. 659
$933 \\ 10 \cdot 2 \cdot 0 \\ 951 \\ 10 \cdot 2 \cdot 2 \\ 953$	1. 0714	3	10. 660
	1. 0451	5	10. 658
	1. 0303	5	10. 658
	1. 0257	3	10. 659
	0. 9939	3	10. 658
10.4.2 $880$ $11.3.1$ $10.6.0$ $11.3.3$	. 9730	1	10. 659
	. 9422	2	10. 660
	. 9312	2	10. 658
	. 9139	3	10. 658
	. 9041	2	10. 659
$10.6.2 \\ 12.0.0 \\ 11.5.1 \\ 12.2.2 \\ 11.5.3$	. 9009 . 8884 . 8792 . 8645 . 8562	3 5 1 1	10. 660 10. 661 10. 660 10. 658 10. 660
$\begin{array}{c} 12.4.0 \\ 991 \\ 10.8.2 \\ 13.1.1 \\ 12.4.4 \end{array}$	. 8428	4	10. 661
	. 8349	2	10. 759
	. 8223	2	10. 658
	. 8151	3	10. 659
	. 8035	3	10. 660
13.3.1	. 7967	2	10. 659

# Cesium Chloroosmate (IV), Cs<sub>2</sub>OsCl<sub>6</sub> (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of cesium chloroosmate was prepared at NBS by R. Johannesen from solutions of cesium chloride and chloroosmic acid. Spectrographic analysis showed the following major impurities: 0.01 to 1.0 percent sodium and 0.001 to 0.01 percent each of aluminum and silicon.

The color of the sample was deep orange. The refractive index could not be determined because the sample was too fine-grained.

The d-values of the three strongest lines are:

3.616, 5.905, and 2.557 A.

Structural data. The structure of cesium chloroosmate has not been reported. However, because of the similarity of patterns, it is thought to be isostructural with ammonium chloroosmate having the space group O<sub>5</sub><sup>6</sup>—Fm3m (No. 225) with 4(Cs<sub>2</sub>OsCl<sub>6</sub>) per unit cell.

Lattice constant

		a
1962	National Bureau of Standards_	A 10.230 at 25 °C.

The density of cesium chloroosmate calculated from the NBS lattice constant is 4.148 g/cm<sup>3</sup> at 25 °C.

hkt	Cu	tional Bureau of 1, 1.5405 A at 2 Internal standangsten, $a=3.16$	25 °C ard,
	d	I	a
111 220 311 222 400	A 5. 905 3. 616 3. 085 2. 953 2. 557	68 100 27 27 27 55	A 10. 228 10. 228 10. 232 10. 228 10. 228
331	2. 347	$\begin{array}{c} 9\\ 37\\ 14\\ 32\\ 12 \end{array}$	10. 230
422	2. 089		10. 230
511	1. 969		10. 231
440	1. 8090		10. 233
531	1. 7293		10. 231
620	1. 6174	14	10. 229
533	1. 5603	3	10. 232
622	1. 5426	3	10. 232
444	1. 4763	8	10. 228
711	1. 4324	7	10. 229
642	1. 3668	13	10. 228
731	1. 3320	3	10. 231
800	1. 2790	3	10. 232
822	1. 2057	5	10. 231
751	1. 1814	2	10. 231
662	1. 1735	2	10. 230
840	1. 1437	4	10. 230
911	1. 1229	2	10. 230
664	1. 0905	3	10. 230
931	1. 0723	2	10. 229
$\begin{array}{c} 844 \\ 933 \\ 10 \cdot 2 \cdot 0 \\ 951 \\ 10 \cdot 2 \cdot 2 \end{array}$	1. 0442	3	10. 231
	1. 0283	1	10. 231
	1. 0032	4	10. 231
	0. 9890	3	10. 230
	. 9843	1	10. 229
$\begin{array}{c} 953 \\ 10 \cdot 4 \cdot 2 \\ 11 \cdot 1 \cdot 1 \\ 880 \\ 11 \cdot 3 \cdot 1 \end{array}$	. 9539 . 9340 . 9225 . 9042 . 8939	${ \begin{array}{c} 1 \\ 3 \\ < 1 \\ 3 \\ 2 \end{array} }$	10. 229 10. 231 10. 231 10. 230 10. 231
$ \begin{array}{c} 10.6.0 \\ 11.3.3 \\ 12.0.0 \\ 12.2.2 \\ 11.5.3 \end{array} $	. 8773	3	10. 231
	. 8678	3	10. 231
	. 8525	3	10. 230
	. 8298	3	10. 230
	. 8218	2	10. 231
$   \begin{array}{c}     12 \cdot 4 \cdot 0 \\     991 \\     10 \cdot 8 \cdot 2 \\     13 \cdot 1 \cdot 1   \end{array} $	. 8088	2	10. 231
	. 8013	2	10. 230
	. 7893	2	10. 230
	. 7823	1	10. 230
Average val	lue of last fiv	ve lines	10. 230

# Chromium Orthophosphate, alpha, CrPO<sub>4</sub> (orthorhombic)

#### Powder Data cards

Card	Index	Radia-	Source
number	lines	tion	
*5-0233	5. 40 2. 74 5. 20	Copper	National Bureau of Standards [1] 1951, [2] 1952.

<sup>\*</sup>This ASTM card was reported without indices.

Additional published patterns. None.

NBS sample. The sample of alpha-chromium orthophosphate was prepared at NBS by grinding the hexahydrate and heating it to 1,500 °C. The ground hexahydrate actually inverts to the alpha form at 972 °C while the unground hexahydrate changes to beta and then to alpha-orthophosphate. Spectrographic analysis showed no impurities greater than 0.001 percent.

The color of the sample was deep blue. The refractive indices are  $N_{\alpha}=1.761$  and  $N_{\gamma}=1.844$ . 2V is very large. The  $\alpha$  form is strongly pleochroic.

The d-values of the three strongest lines are: 5.390, 2.741, and 5.203 A.

Structural data. Villadsen [3] in 1960 determined that alpha-chromium orthophosphate has an orthorhombic body-centered lattice having the lattice symbol I . . . . Therefore, the possible orthorhombic space groups are D<sub>2</sub><sup>8</sup>—I222 (No. 23),  $D_2^9 - I_{2_1} 2_{1_2} 1_{1_2} 1_{1_3} 1_{1_4} 1_{1_5} 1_{1$  $D_{2h}^{25}$ —Immm (No. 71). According to Villadsen, there are either 8(CrPO<sub>4</sub>) per unit cell or 16(CrPO<sub>4</sub>) per unit cell.

Lattice constants

		a	b	c
1960 1962	Villadsen [3] National Bureau of Standards.	A 10. 41 10. 405	A 12. 90 12. 898	$A \\ 6.297 \\ 6.297 \text{ at} \\ 25 \ ^{\circ}\text{C}$

The density of alpha-chromium orthophosphate calculated from the NBS lattice constants using Z=16 is 4.620 g/cm³ at 25 °C. The density based on Z=8 appeared to be rather low for this compound.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A		
	d	I	
020 011 101 200 121	A 6. 444 5. 661 5. 390 5. 203 4. 139	17 45 100 48 4	
211 031 002 301 022	3. 834 3. 548 3. 149 3. 039 2. 826	$\begin{array}{c} 3 \\ 7 \\ 9 \\ 22 \\ 2 \end{array}$	
141 240 202 400 222	2. 766 2. 741 2. 693 2. 604 2. 479	13 51 40 26 7	
251 013 440 213 303	2. 169 2. 071 2. 025 1. 927 1. 795	18 5 13 5 3	
451 323 442 547 370	1. 7590 1. 7296 1. 7025 1. 6851 1. 6276	8 3 13 3 4	
080 004 253 433 602	1. 6124 1. 5754 1. 5537 1. 5269 1. 5188	5 6 3 8 6	
204 372 651 453 244	1. 5071 1. 4457 1. 4031 1. 3801 1. 3649	3 2 4 8 3	
291	1. 3493	3	

#### References

- [1] Joint Committee Fellowship Report, National Bureau
- of Standards, Oct., 1951.
  [2] B. M. Sullivan and H. F. McMurdie, Crystal forms of chromium orthophosphate, J. Research N.B.S. 48, No. 2, 159–162 (1952) RP2300.
  [3] J. Villadsen, Halder Topsoe Res. Lab., Hellerup, Den-
- mark (private communication).

# Cobalt Mercury Thiocyanate, Co[Hg(CNS)<sub>4</sub>] (tetragonal)

Powder Data cards. None.

NBS sample. The sample of cobalt mercury thiocyanate was prepared at NBS by R. S. Johannesen from solutions of cobaltous nitrate and ammonium mercury thiocyanate. Spectrographic analysis showed the following major impurities: 0.001 to 0.01 percent each of nickel and silicon.

The color of the sample was a brilliant blue and it is optically positive. The indices of refraction are  $N_o = 1.875$  and  $N_e = 1.905$ .

The d-values of the three strongest lines are:

5.552, 3.284, and 7.85 A.
Structural data. Straumanis and Stahl [1] in 1944 determined that cobalt mercury thiocyanate has the space group  $S_4^2 - \overline{I4}$  (No. 82) and 2{Co[Hg(CNS)<sub>4</sub>]} per unit cell.

Unit cell measurements reported by Straumanis and Stahl have been converted from kX to angstrom units for comparison with the NBS

values.

Lattice constants

		<i>a</i>	c
1944	Straumanis and Stahl [1].	$A \\ 11. 1092$	$\begin{array}{c} A \\ 4.\ 3740 \end{array}$
1947 1962	Jeffrey [2] National Bureau of Standards.	11. 09 11. 105	4. 37 4. 3819 at 25 °C

Straumanis and Stahl [1] reported that the thermal expansion coefficients for cobalt mercury thiocyanate were:  $\alpha \perp c = -10.85 \times 10^{-6}$ ,  $\alpha \parallel c =$  $149.3 \times 10^{-6}$ .

The density of cobalt mercury thiocyanate calculated from the NBS lattice constants is  $3.022 \text{ g/cm}^3 \text{ at } 25 \text{ °C}.$ 

#### References

[1] I. M. Straumanis and W. Stahl, Die gegenseitige Löslichkeit im ternären System Cadmium-, Kobalt-, Zinkquecksilberrhodanid, Z. physik. Chem. 193, 97-111 (1944)

[2] J. W. Jeffrey, Crystal structure of Co[Hg(CNS)<sub>4</sub>], Nature **159**, 610 (1947).

<u> </u>			
hkl	of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	I	
110 200 101 220 310	A 7. 85 5. 552 4. 075 3. 992 3. 513	100 100 44 41 18	
211 301 400 330 321	3. 284 2. 828 2. 776 2. 617 2. 520	$70 \\ 44 \\ 6 \\ 19 \\ 39$	
420 411 510 501 440	2. 484 2. 295 2. 177 1. 980 1. 962	32 25 5 19 11	
530 521 600 620 402	1. 903 1. 865 1. 850 1. 755 1. 721	$\begin{bmatrix} 7 \\ 23 \\ 14 \\ 10 \\ 4 \end{bmatrix}$	
611 541 710 631 512	1. 683 1. 6122 1. 5700 1. 5482 1. 5442	11 5 5 12 11	
640 701 721 800 651	1. 5396 1. 4916 1. 4403 1. 3880 1. 3523	5 2 7 2 4	
820 811 660 831 840	1. 3466 1. 3143 1. 3090 1. 2464 1. 2414	3 5 3 2 2	
910 921 851 10·0·0 941	1. 2267 1. 1616 1. 1369 1. 1104 1. 0921	2 3 1 2 2	
$ \begin{array}{c} 10 \cdot 2 \cdot 0 \\ 950 \\ 10 \cdot 1 \cdot 1 \\ 10 \cdot 4 \cdot 0 \end{array} $	1. 0890 1. 0784 1. 0719 1. 0315	2 2 3 2	

#### Powder Data Cards

Card number	Index	Radiation	Source
3-0843	2. 58 3. 60 4. 30	Molybde- num	The Dow Chemical Company.

Additional published patterns. Hammel [1] 1938, Rentzeperis [2] 1958, and Pistorius [3] 1961. The reference for the comprehensive work reported by Pistorius was not available at the time this work was started. The d-values reported by Pistorius agree favorably with the NBS data.

NBS sample. The sample of cobalt sulfate was made from cobalt chloride and sulfuric acid. The precipitated sulfate was heated to 160 °C to drive off excess sulfuric acid. A second pattern was prepared after the sample was reheated to 400 °C with no observable change in spacing. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of nickel and silicon; and 0.01 to 0.1 percent each of aluminum, calcium, iron, and sodium.

The color of the sample was reddish-purple. The indices of refraction could not be determined because the sample was too fine-grained.

The d-values of the three strongest lines are:

2.605, 3.610, and 3.368 A.

Structural data. Rentzeperis [2] in 1958 determined that beta cobalt sulfate has the magnesium sulfate structure, the space group  $D_{2h}^{17}$ —Amam (No. 63) and  $4(\text{CoSO}_4)$  per unit cell. Hammel [1] and Hocart and Serres [4] both had previously reported lattice constants for what was later found to be the high-temperature  $\alpha\text{-CoSO}_4$  reported by Rentzeperis [2] to exist after heating above 700 °C.

Lattice constants

		a	b	c
1958	Rentzeperis [2]	A 6. 531	A 7. 876	A 5. 200
1961	Pistorius [3]	6. 516	7. 864	5. 191 at 25 °C
1962	National Bureau of Standards.	6. 522	7. 871	5. 198 at 25 °C

The density of beta-cobalt sulfate calculated from the NBS lattice constants is 3.857 g/cm<sup>3</sup> at 25 °C.

hkl	1962 National Bureau of Standards Co, 1.7889 A at 25 °C Internal standard, tungsten, a=3.1648 A	
011 020 111 120 211 031 202 040 320, 231 222	A 4. 336 3. 936 3. 610 3. 368 2. 605 2. 342 2. 032 1. 967 1. 902 1. 805	28 21 67 45 100 38 19 12 10 21
240 113 400 331 411	1. 684 1. 6379 1. 6305 1. 5938 1. 5261	13 18 12 7 10
$\begin{array}{c} 420,051 \\ 213 \\ 033 \\ 242 \\ 251 \end{array}$	1. 5066 1. 5023 1. 4460 1. 4140 1. 3680	$12 \\ 5 \\ 10 \\ 22 \\ 10$
431	1. 3383	10

#### References

[1] F. Hammel, Contribution à l'étude des sulfates de la série magnésienne, Ann. chim. (Paris) **11**, 24–358 (1938).

[2] P. J. Rentzeperis, Die Kristallstruktur der beiden Modifikationen von wasserfreiem CoSO<sub>4</sub>, Neues. Jahrb. Mineral. Monatsh. 210–215 (1958).

[3] C. W. F. T. Pistorius, Lattice constants and space groups of the low and high temperature polymorphic forms of anhydrous cobaltous sulfate, Acta Cryst. 14, 543-544 (1961)

14, 543-544 (1961).
[4] R. Hocart and A. Serres, Magnetic properties and crystalline structure in the different varieties of anhydrous cobalt sulfate, Compt. rend. 193, 1180-1182 (1931).

# Dysprosium Gallium Oxide 3:5, Dy<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub> (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of dysprosium oxide and gallium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hr; then ground, remixed, and again pressed into pellets and heated at 1,450 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent holmium; 0.001 to 0.01 percent each of erbium, thulium, and yttrium; and 0.0001 to 0.001 percent each of copper and silicon.

The color of the sample was white. The index of refraction could not be determined because the

sample was too fine-grained.

The d-values of the three strongest lines are

2.752, 2.512, and 1.645 A.

Structural data. S. Schneider and R. Roth [1] showed that dysprosium gallium oxide 3:5 has the garnet structure, having the space group O<sub>h</sub><sup>10</sup>—Ia3d (No. 230), and 8[Dy<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub>] per unit cell.

#### Lattice constants

1956 1962	Bertaut and Forrat [2] National Bureau of Standards_	A 12.32 12.307 at 25 °C
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The density of dysprosium gallium oxide 3:5 calculated from the NBS lattice constant is 7.325 g/cm<sup>3</sup> at 25 °C.

#### References

[1] S. Schneider and R. Roth, Solid state reactions involving oxides of trivalent cations (to be published in J. Research NBS).

[2] F. Bertaut and F. Forrat, Étude des combinaisons des oxides des terres rares avec l'alumine et la galline, Compt. rend. **243**, 1219–1222 (1956).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, a=4.0861 A		
	d	I	a
211 220 321 400 420	A 5. 023 4. 350 3. 290 3. 076 2. 752	14 6 10 30 100	A 12. 304 12. 304 12. 310 12. 304 12. 307
422	2. 512	44	12. 306
431	2. 413	5	12. 304
521	2. 247	10	12. 307
440	2. 176	2	12. 309
611	1. 997	9	12. 310
444	1. 777	14	12. 311
640	1. 707	32	12. 309
721	1. 675	6	12. 308
642	1. 645	36	12. 308
732	1. 564	4	12. 311
800	1, 5382	14	12. 306
822	1, 4503	5	12. 306
840	1, 3760	9	12. 307
842	1, 3430	20	12. 310
921	1, 3271	1	12. 307
664	1. 3120	7	12. 308
932	1. 2695	3	12. 308
10·2·0	1. 2068	4	12. 307
10·3·1	1. 1737	2	12. 310
10·4·0	1. 1426	17	12. 306
$ \begin{array}{c} 10 \cdot 3 \cdot 3 \\ 10 \cdot 4 \cdot 2 \\ 11 \cdot 2 \cdot 1 \\ 880 \\ 12 \cdot 0 \cdot 0 \end{array} $	1. 1330	<1	12. 308
	1. 1235	9	12. 307
	1. 0967	3	12. 310
	1. 0880	7	12. 309
	1. 0256	6	12. 307
$\begin{array}{c} 12 \cdot 2 \cdot 0 \\ 12 \cdot 2 \cdot 2 \\ 12 \cdot 4 \cdot 4 \\ 13 \cdot 3 \cdot 0 \\ 12 \cdot 6 \cdot 0 \end{array}$	1. 0117	5	12. 308
	0. 9983	9	12. 308
	. 9278	3	12. 309
	. 9228	2	12. 312
	. 9173	11	12. 307
12.6.2	. 9073	5	12. 307
888	. 8881	4	12. 306
14.3.1	. 8576	3	12. 309
12.8.0	. 8534	2	12. 308
14.4.0	. 8452	10	12. 306
14.4.2	. 8373	9	12. 307

# Erbium Manganite, ErMnO<sub>3</sub> (hexagonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of erbium manganite was prepared at NBS by S. Schneider from stoichiometric mixtures of erbium oxide and manganous carbonate. The mixture was pressed into pellets and heated at 1,000 °C for 41 hr; then ground, remixed, again pressed into pellets and heated at 1,150 °C for 21 hr. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum and magnesium; and 0.001 to 0.01 percent each of calcium, chromium, copper, iron, and silicon.

The sample was a black opaque powder. The d-values of the three strongest lines are: 2.695,

3.059, and 1.7659 A. Structural data. Yakel, Koehler, Bertaut, and Forrat [1] in 1960 determined that erbium manganite has the space group C<sub>6v</sub><sup>3</sup>-P<sub>63</sub>cm (No. 185), and 6(ErMnO<sub>3</sub>) per unit cell. Erbium manganite is isostructural with lutetium manganite.

Lattice constants

		a	с
1960	Yakel, Koehler, Ber- taut, and Forrat [1].	A 6. 1150	$A \ 11.411$
1962	National Bureau of Standards.	6. 1166	11.435 at 25 °C.

The density of erbium manganite calculated from the NBS lattice constants is 7.264 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] H. L. Yakel, W. C. Koehler, E. F. Bertaut, and E. F. Forrat, Erbium Manganite—a new ABO<sub>3</sub> structure, Acta Cryst. 13, 1015 (1960).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	I
002 102 110 111 004	A 5. 717 3. 885 3. 059 2. 955 2. 858	30 9 50 33 35
112 104 202 113 114	2. 695 2. 516 2. 403 2. 385 2. 088	100 7 6 3 38
204 212 115 106 300	1. 944 1. 8900 1. 8312 1. 7931 1. 7659	6 4 6 10 40
302 214 116 206 220	1. 6874 1. 6396 1. 6170 1. 5470 1. 5290	9 5 19 5 7
221 304 222 117 008	1. 5156 1. 5023 1. 4769 1. 4409 1. 4298	4 25 16 3 2
108 224 314 225 208	1. 3801 1. 3481 1. 3067 1. 2714 1. 2576	9 7 2 2 2 2
226 218,316 410 411 412	1. 1926 1. 1636 1. 1558 1. 1506 1. 1330	5 5 4 1 9
324 1.0.10 308 406 414	1. 1184 1. 1178 1. 1109 1. 0876 1. 0715	5 4 3 <1 8
$\begin{array}{c} 2.0.10 \\ 228 \\ 415 \\ 318, 326 \\ 330 \end{array}$	1. 0499 1. 0444 1. 0315 1. 0245 1. 0193	1 <1 1 5 4
$ \begin{array}{r} 332 \\ 2 \cdot 1 \cdot 10 \\ 416 \\ 408 \\ 334 \end{array} $	1. 0037 0. 9930 . 9883 . 9715 . 9602	2 3 4 1 3
417 335 3·1·10	. 9433 . 9314 . 9023	$\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix}$

# Europium Gallium Oxide 3:5, Eu<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub> (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of europium oxide and gallium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hr; then ground, remixed, again pressed into pellets and heated at 1,450 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent silicon; and 0.0001 to 0.001 percent each of barium, calcium, and erbium.

The color of the sample was white. The index of refraction was above 2.0 as determined by the available refractive index liquids.

The d-values of the three strongest lines are:

2.773, 2.531, and 1.6573 A.

Structural data. Schneider, Roth, and Waring [1] in 1961 showed that europium gallium oxide 3:5 has the garnet structure, having the space group O<sub>10</sub><sup>10</sup>—Ia3d (No. 230), and 8[Eu<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub>] per unit cell.

#### Lattice constant

1962	National Bureau of Standards_	
1002		25 °C

The density of europium gallium oxide 3:5 calculated from the NBS lattice constant is 6.940 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] S. J. Schneider, R. S. Roth, and J. L. Waring, Solid state reactions involving oxides of trivalent cations, J. Research NBS **65A** (Phys. and Chem.) No. 4, 345-374 (1961).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, tungsten, $a=3.1648$ A		5 °C
	d	I	a
211 220 321 400 420	A 5. 063 4. 384 3. 314 3. 099 2. 773	14 5 8 32 100	A 12. 402 12. 400 12. 400 12. 396 12. 401
422 431 521 440 611	2. 531 2. 432 2. 264 2. 192 2. 012	45 3 10 4 11	12. 399 12. 401 12. 400 12. 400 12. 403
$631 \\ 444 \\ 640 \\ 721 \\ 642$	1. 829 1. 790 1. 7196 1. 6874 1. 6573	$egin{array}{c} 1 \\ 14 \\ 30 \\ 4 \\ 35 \end{array}$	12. 405 12. 402 12. 400 12. 400 12. 402
732 800 840 842 921	1. 5749 1. 5504 1. 3866 1. 3534 1. 3374	5 13 9 17 3	12. 401 12. 403 12. 402 12. 404 12. 403
$\begin{array}{c} 664 \\ 932 \\ 941 \\ 10 \cdot 2 \cdot 0 \\ 10 \cdot 3 \cdot 1 \end{array}$	1. 3224 1. 2796 1. 2531 1. 2162 1. 1827	7 2 1 1 2	12. 405 12. 406 12. 405 12. 405 12. 404
$   \begin{array}{c}     10.4.0 \\     10.4.2 \\     11.2.1 \\     880 \\     11.3.2   \end{array} $	1. 1517 1. 1323 1. 1049 1. 0962 1. 0713	17 8 3 6 2	12. 404 12. 403 12. 403 12. 402 12. 401
$ \begin{array}{c} 12.0.0 \\ 12.2.0 \\ 11.5.2 \\ 12.2.2 \\ 11.6.1 \end{array} $	1. 0336 1. 0196 1. 0128 1. 0060 0. 9867	3 5 3 7 3	12. 403 12. 404 12. 404 12. 403 12. 403
$ \begin{array}{r} 11.6.3 \\ 12.4.4 \\ 12.6.0 \\ 13.3.2 \\ 12.6.2 \end{array} $	. 9627 . 9349 . 9244 . 9194 . 9142	$ \begin{array}{c} <1\\ 5\\ 10\\ <1\\ 5 \end{array} $	12. 403 12. 403 12. 402 12. 403 12. 401
888 14·3·1 12·8·0 14·4·0 14·4·2	. 8951 . 8640 . 8599 . 8517 . 8438	5 3 5 8 16	12. 403 12. 401 12. 402 12. 401 12. 401
14.5.1	. 8323	1	12. 401
Average va	lue of last five	lines	12. 401

# Gadolinium Gallium Oxide 3:5, Gd<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub> (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of gadolinium oxide and gallium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hrs; then ground, remixed, and again pressed into pellets and heated at 1,450 °C for 6 hrs. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of europium and terbium; and 0.001 to 0.01 percent of silicon.

The color of the sample was white. The index

of refraction is greater than 2.00.

The d-values of the three strongest lines are:

2.768, 2.526, and 1.6540 A.

Structural data. S. Schneider and R. Roth [1] showed that gadolinium gallium oxide 3:5 has the garnet structure, having the space group  $O_h^{10}$ —Ia3d (No. 230), and  $8[Gd_3Ga_2(GaO_4)_3]$  per unit cell.

#### Lattice constants

1956 Be 1962 Na	rtaut and Forrat [2] tional Bureau of Standards_	A 12.39 12.376 at 25 °C
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The density of gadolinium gallium oxide 3:5 calculated from the NBS lattice constant is 7.093 g/cm³ at 25 °C.

#### References

[1] S. Schneider and R. Roth, Solid state reactions involving oxides of trivalent cations (to be published in J. Research NBS).

[2] F. Bertaut and F. Forrat, Étude des combinaisions des oxides des terres rares avec l'alumine et la galline, Compt. rend. **243**, 1219–1222 (1956).

hkl	Cu, 1.5	nal Bureau of $5405$ A at $25$ ernal Standar sten, $a=3.16$	o°C cd,
	d	I	<i>a</i> .
211 220 321 400 420	A 5. 052 4. 375 3. 307 3. 094 2. 768	15 8 10 32 100	A 12. 375 12. 374 12. 374 12. 376 12. 379
422	2. 526	42	12. 375
431	2. 428	5	12. 380
521	2. 259	21	12. 373
440	2. 188	6	12. 377
611	2. 0077	10	12. 376
444	1. 7865	14	12. 377
640	1. 7160	32	12. 374
721	1. 6842	7	12. 376
642	1. 6540	36	12. 377
732	1. 5720	3	12. 378
800	1. 5468	13	12. 374
840	1. 3837	10	12. 376
842	1. 3503	20	12. 376
921	1. 3348	3	12. 378
664	1. 3193	6	12. 376
$   \begin{array}{c}     10 \cdot 2 \cdot 0 \\     10 \cdot 3 \cdot 1 \\     10 \cdot 4 \cdot 0 \\     10 \cdot 3 \cdot 3 \\     10 \cdot 4 \cdot 2   \end{array} $	1. 2138	5	12. 378
	1. 1800	5	12. 376
	1. 1491	15	12. 376
	1. 1392	2	12. 375
	1. 1297	10	12. 375
$ \begin{array}{c} 11 \cdot 2 \cdot 1 \\ 880 \\ 12 \cdot 0 \cdot 0 \\ 12 \cdot 2 \cdot 0 \\ 12 \cdot 2 \cdot 2 \end{array} $	1. 1025	5	12. 376
	1. 0938	6	12. 375
	1. 0315	7	12. 378
	1. 0173	8	12. 376
	1. 0038	10	12. 376
$   \begin{array}{c}     11 \cdot 6 \cdot 3 \\     12 \cdot 4 \cdot 4 \\     12 \cdot 6 \cdot 0 \\     12 \cdot 6 \cdot 2 \\     888   \end{array} $	0. 9603	3	12. 373
	. 9328	5	12. 375
	. 9224	9	12. 375
	. 9123	6	12. 375
	. 8931	7	12. 375
14·3·1	. 8623	3	12. 376
12·8·0	. 8581	3	12. 376
14·4·0	. 8500	8	12. 376
14·4·2	. 8422	8	12. 378
Average va	alue of last five	lines	12. 376

# Lithium Arsenate, Li<sub>3</sub>AsO<sub>4</sub> (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium arsenate was prepared at NBS by reaction of solutions of lithium carbonate and arsenic (V) acid. The precipitate was washed and then heated to 1,000 °C for 10 min. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent each of antimony and lead; 0.01 to 0.1 percent each of aluminum, bismuth, calcium, magnesium, and silicon.

The sample was colorless. The refractive indices were not determined because the particle size of the sample was too small.

The d-values of the three strongest lines are:

3.89, 4.09, and 3.643 A.

Structural data. Zemann [1] in 1960 determined that lithium arsenate is probably isotypic with lithium phosphate, with the olivine structure, the space group D<sub>2h</sub><sup>16</sup>—Pmnb (No. 62), and 4(Li<sub>3</sub>AsO<sub>4</sub>) per unit cell.

Lattice constant

		a	b	c
1962	National Bureau of Standards.	6. 279	A 10. 768	A 4.955 at 25 °C

The density of lithium arsenate calculated from the NBS lattice constants is 3.166 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] J. Zemann, Die Kristallstruktur von Lithiumphosphat, Li<sub>3</sub>PO<sub>4</sub>, Acta Cryst. 13, 863-867 (1960).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	I
020 120 101 021 121	A 5. 39 4. 09 3. 89 3. 643 3. 151	$   \begin{array}{r}     36 \\     99 \\     100 \\     69 \\     45   \end{array} $
200 220 040 140, 002 221	3. 141 2. 712 2. 692 2. 476 2. 377	$ \begin{array}{c} 46 \\ 52 \\ 31 \\ 48 \\ 227 \end{array} $
$\begin{array}{c} 041 \\ 022 \\ 141 \\ 122 \\ 240 \end{array}$	2. 366 2. 249 2. 213 2. 118 2. 043	16 4 11 19 2
320 202 301 241 222	1. 950 1. 945 1. 927 1. 889 1. 828	12 12 9 16 15
$\begin{array}{c} 042 \\ 321 \\ 060 \\ 142 \\ 160 \end{array}$	1. 824 1. 8151 1. 7944 1. 7502 1. 7256	13 10 5 7 2
061 340 161 103 023	1. 6871 1. 6521 1. 6294 1. 5975 1. 5788	
242 400 260 322 420	1, 5761 1, 5695 1, 5582 1, 5322 1, 5071	$egin{array}{c} 7 \\ 14 \\ 22 \\ 7 \\ 2 \end{array}$
062 421 223 342 440	1. 4539 1. 4419 1. 4104 1. 3746 1. 3561	$\begin{array}{c} 3 \\ 6 \\ 16 \\ 6 \\ 3 \end{array}$
080 402 262 180, 412 361	1, 3462 1, 3261 1, 3190 1, 3158 1, 3139	$ \begin{array}{c} <1 \\ 6 \\ 12 \\ 12 \\ 10 \end{array} $
081 303	1. 2986 1. 2968	3 3

# Lithium Trimetaphosphate Trihydrate, Li<sub>3</sub>P<sub>3</sub>O<sub>3</sub>•3H<sub>2</sub>O (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium trimetaphosphate trihydrate was prepared at NBS by E. D. Eanes by adding an excess amount of AgNO<sub>3</sub> to a solution of Na<sub>3</sub>P<sub>3</sub>O<sub>9</sub>·1½H<sub>2</sub>O. A slurry of the silver salt was metathesized with LiCl. After filtering to remove AgCl, the product was precipitated from solution with ethanol. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of calcium, barium, and sodium; and 0.001 to 0.01 percent each of aluminum, lead, magnesium, and silicon.

The sample is colorless and optically positive. The indices of refraction are N<sub>o</sub>=1.468, and

 $N_e = 1.472$ .

The d-values of the three strongest lines are:

4.965, 3.128, and 6.24 A.

Structural data. The structure of lithium trimetaphosphate trihydrate was determined by E. D. Eanes [1] in 1961 at NBS. The space group is  $C_{3v}^{5}$ —R3m (No. 160) and  $3(\text{Li}_{3}P_{3}O_{9}3H_{2}O)$  per hexagonal unit cell or 1(Li<sub>3</sub>P<sub>3</sub>O<sub>9</sub>·3H<sub>2</sub>O) per rhombohedral unit cell.

Lattice constant

1962	National Bureau of	<i>a A</i> 12. 513	c A 5. 5900
1302	Standards.	12. 515	at 25 °C

The density of lithium trimetaphosphate trihydrate calculated from the NBS lattice constants is  $2.048 \text{ g/cm}^3$  at 25 °C.

#### Reference

[1] E. D. Eanes and H. Ondik, The structure of lithium dipotassium trimetaphosphate monohydrate, Acta Cryst. 15, 1280-1285 (1962).

hkl (hex)	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A	
	d	I
110 101 021 300 211	A 6. 24 4. 965 3. 889 3. 610 3. 302	51 100 37 13 38
220	3. 128	66
012	2. 706	23
131	2. 647	29
202	2. 483	3
401	2. 437	8
410	2. 365	11
122	2. 309	7
321	2. 272	9
330	2. 085	10
312	2. 047	2
$051 \\ 042 \\ 241 \\ 003, 232 \\ 511$	2. 021 1. 947 1. 924 1. 858 1. 838	$<_{1}^{2}$ $<_{7}^{8}$ $_{3}^{8}$
600	1. 805	2
113	1. 786	6
520	1. 736	5
502	1. 712	1
431	1. 698	2
303	1. 657	1
422	1. 652	4
223	1. 601	3
152	1. 598	3
161	1. 585	5
440	1. 564	1
342	1. 502	2
701	1. 491	3
413	1. 4635	5
621	1. 4513	3
710	1. 4355	4
612	1. 4227	2
333	1. 3895	2
104	1. 3857	3
630	1. 3652	2
072 541	1. 3544 1. 3469	$\begin{bmatrix} 2 \\ 2 \end{bmatrix}$

# Lithium Tungstate Hemihydrate, Li<sub>2</sub>WO<sub>4</sub>·½H<sub>2</sub>O (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lithium tungstate hemihydrate was obtained from the City Chemical Company, New York, N.Y. Upon fusion this substance loses 3.18 percent water and converts to the anhydrous trigonal form. Spectrographic

analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, copper, iron, lead, molybdenum, and silicon.

The sample was colorless. The refractive index was not determined because the particle size was too small.

The d-values of the three strongest lines are: 4.81, 2.774, and 3.398 A.

# Lithium Tungstate Hemihydrate, Li<sub>2</sub>WO<sub>4</sub> • ½H<sub>2</sub>O (cubic)—Continued

Structural data. No reference was found for the structure of this compound. The lattice is apparently primitive cubic and the unit cell probably contains  $6(\text{Li}_2\text{WO}_4\cdot\frac{1}{2}\text{H}_2\text{O})$ .

The density of lithium tungstate hemihydrate calculated from the NBS lattice constant is 4.682 g/cm³ at 25 °C. The average pycnometric density was approximately 4.3 g/cm³ at 25 °C.

#### Lattice constant

1962	National Bureau of Standards_	8.3203 at 25 °C

hkl	Cu,1	mal Bureau of5405 A at 25 ternal standar sten, $a=3.16$	5 °C cd,
	đ	I	а
100 110 111 200 210	A 8. 32 5. 89 4. 81 4. 16 3. 723	47 8 100 15 30	A 8. 32 8. 33 8. 33 8. 32 8. 325
211	3. 398	81	8. 323
220	2. 942	30	8. 321
300	2. 774	82	8. 322
310	2. 631	38	8. 320
311	2. 509	9	8. 321
222	2. 402	13	8. 321
321	2. 224	11	8. 321
400	2. 080	11	8. 320
410	2. 018	33	8. 320
411	1. 9612	16	8. 3207
331	1. 9091	$   \begin{array}{c}     37 \\     21 \\     6 \\     4 \\     12   \end{array} $	8. 3216
420	1. 8606		8. 3209
421	1. 8155		8. 3197
332	1. 7739		8. 3209
422	1. 6984		8. 3204
500	1. 6642	10	8. 3210
510	1. 6316	5	8. 3196
511	1. 6014	10	8. 3211
520	1. 5449	7	8. 3195
521	1. 5190	20	8. 3199
440	1. 4708	24	8. 3201
522	1. 4485	14	8. 3210
530	1. 4269	10	8. 3202
531	1. 4065	13	8. 3210
600	1. 3868	7	8. 3208
611	1. 3498	8	8. 3207
620	1. 3157	3	8. 3212
621	1. 2994	13	8. 3202
541	1. 2837	2	8. 3193
533	1. 2689	2	8. 3207

hkl	Inte	al Bureau of $5405$ A at $25$ ernal standar ten, $a=3.164$	5 °C. cd,
	d	1	a
A	A	$\begin{array}{c} 5 \\ 7 \\ 5 \\ < 1 \\ 2 \end{array}$	A
622	1. 2544		8. 3207
630	1. 2403		8. 3202
631	1. 2268		8. 3206
444	1. 2010		8. 3208
700	1. 1887		8. 3209
710	1. 1766	3	8. 3198
711	1. 1651	9	8. 3205
720	1. 1428	4	8. 3197
721	1. 1323	7	8. 3207
642	1. 1118	6	8. 3199
722	1. 1022	2	8. 3214
730	1. 0924	5	8. 3195
731	1. 0832	2	8. 3202
650	1. 0653	2	8. 3203
732	1. 0567	4	8. 3205
800	1. 0401	3	8. 3208
810	1. 0320	10	8. 3203
811	1. 0242	6	8. 3206
733	1. 0166	7	8. 3212
820	1. 0090	6	8. 3204
821	1. 0017	3	8. 3207
653	0. 9946	2	8. 3214
822	. 9805	6	8. 3198
830	. 9738	2	8. 3202
831	. 9673	4	8. 3210
751	. 9608	3	8. 3208
662	. 9545	2	8. 3211
832	. 9481	2	8. 3195
900	. 9245	4	8. 3205
911	. 9133	6	8. 3206
842	. 9078	$\begin{array}{c} 4 \\ 1 \\ 6 \\ 1 \\ 4 \end{array}$	8. 3201
920	. 9024		8. 3197
921	. 8973		8. 3212
664	. 8869		8. 3199
922	. 8820		8. 3208
930	. 8771	2	8. 3209
931	. 8722	3	8. 3203
852	. 8628	3	8. 3205
932	. 8582	5	8. 3206
844	. 8492	6	8. 3204
$\begin{array}{c} 940 \\ 941 \\ 933 \\ 10 \cdot 0 \cdot 0 \\ 10 \cdot 1 \cdot 0 \end{array}$	. 8448 . 8405 . 8362 . 8320 . 8279	$\begin{array}{c} 3 \\ 2 \\ 6 \\ 2 \\ 7 \end{array}$	8. 3203 8. 3205 8. 3201 8. 3200 8. 3203
10.1.1	. 8239	1	8. 3206

# Lutetium Gallium Oxide 3:5, Lu<sub>3</sub>Ga<sub>2</sub>(GaO<sub>4</sub>)<sub>3</sub> (cubic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample was prepared at NBS by S. Schneider from stoichiometric mixtures of gallium oxide and lutetium oxide. The mixture was pressed into pellets and heated at 1,350 °C for 6 hr; then ground, remixed, and again pressed into pellets and heated at 1,450 °C for 6 hr. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of erbium and silicon; and 0.0001 to 0.001 percent each of dysprosium, yttrium, and ytterbium.

The color of the sample was white. The index of refraction could not be determined because

the sample was too fine-grained.

The d-values of the three strongest lines are:

2.724, 2.487, and 1.628 A.
Structural data. S. Schneider and R. Roth [1] showed that lutetium gallium oxide has the garnet structure, having the space group O<sup>10</sup><sub>h</sub>—Ia3d (No. 230), and  $8[La_3Ga_2(GaO_4)_3]$  per unit cell.

#### Lattice constant

1962	National ards.	Bureau	of	Stand-	$^{A}_{12.183}$ at $^{26}$ °C

The density of lutetium gallium oxide 3:5 calculated from the NBS lattice constant is 7.826 g/cm³ at 26 °C.

#### Reference

[1] S. Schneider and R. Roth, Solid state reactions involving oxides of trivalent cations (to be published in J. Research NBS).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A				
	d	I	a		
211 220 321 400 420 422 510 521 440 611 631 444 640 721 642 732 800 653 822 752	A 4. 973 4. 308 3. 256 3. 046 2. 724 2. 487 2. 389 2. 224 2. 154 1. 976 1. 758 1. 689 1. 658 1. 658 1. 628 1. 547 1. 523 1. 456 1. 436 1. 3797	19 6 12 31 100 44 3 13 3 12 2 17 32 6 34 3 14 2 2	A 12. 181 12. 185 12. 183 12. 184 12. 182 12. 184 12. 182 12. 181 12. 185 12. 181 12. 180 12. 180 12. 184 12. 181 12. 184 12. 181 12. 185 12. 181 12. 185 12. 181		
840	1. 3620	8	12. 182		
842	1. 3291	21	12. 181		
921	1. 3138	2	12. 184		
664	1. 2986	7	12. 182		
932	1. 2566	2	12. 183		
$10 \cdot 1 \cdot 1$ $10 \cdot 2 \cdot 0$ $10 \cdot 3 \cdot 1$ $10 \cdot 4 \cdot 0$ $10 \cdot 3 \cdot 3$	1. 2063	1	12. 183		
	1. 1947	2	12. 184		
	1. 1617	3	12. 184		
	1. 1311	20	12. 182		
	1. 1215	2	12. 183		
$\begin{array}{c} 10 \cdot 4 \cdot 2 \\ 11 \cdot 2 \cdot 1 \\ 880 \\ 11 \cdot 3 \cdot 2 \\ 10 \cdot 6 \cdot 0 \end{array}$	1. 1120	7	12. 181		
	1. 0853	3	12. 182		
	1. 0768	8	12. 183		
	1. 0523	2	12. 181		
	1. 0447	2	12. 183		
$12.0.0 \\ 12.2.0 \\ 11.5.2 \\ 12.2.2 \\ 11.6.1$	1. 0151 1. 0014 0. 9947 . 9881 . 9691	5 5 1 8	12. 181 12. 183 12. 183 12. 182 12. 181		
11.6.3 $13.2.1$ $12.4.4$ $12.6.0$ $13.3.2$	. 9455	<1	12. 182		
	. 9235	1	12. 181		
	. 9183	6	12. 183		
	. 9080	12	12. 182		
	. 9031	1	12. 183		
$\begin{array}{c} 12 \cdot 6 \cdot 2 \\ 888 \\ 14 \cdot 1 \cdot 1 \\ 14 \cdot 2 \cdot 0 \\ 14 \cdot 3 \cdot 1 \end{array}$	. 8981	5	12. 182		
	. 8792	5	12. 183		
	. 8657	1	12. 181		
	. 8615	1	12. 184		
	. 8488	2	12. 183		
12.8.0 $14.4.0$ $14.4.2$	. 8447	4	12. 182		
	. 8368	12	12. 184		
	. 8289	10	12. 182		
Average va	lue of last five	lines	12. 183		

# Lutetium Manganite, LuMnO<sub>3</sub> (hexagonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of lutetium manganite was prepared at NBS by S. Schneider from stoichiometric mixtures of lutetium oxide and manganous carbonate. The mixture was pressed into pellets and heated at 1,000 °C for 41 hr then reheated at 1,150 °C for 21 hr. Spectrographic analysis showed the following major impurities: 0.01 to 0.1 percent each of calcium and magnesium; and 0.001 to 0.01 percent each of aluminum and silicon.

The sample was a black opaque powder. The d-values of the three strongest lines are:

2.668, 3.022 and 1.7449A.

Structural data. Yakel, Koehler, Bertaut, and Forrat [1] in 1960 determined that lutetium manganite has the space group  $C_{6v}^3$ — $P6_3$ cm (No. 185), and  $6[LuMnO_3]^5$  per unit cell.

hkl	of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A			
	d	I		
02	5. 694	34		
002	3. 851	11		
110	3. 022	53		
111	2. 922	26		
004	2. 848	29		
$   \begin{array}{r}     112 \\     104 \\     202 \\     114 \\     204   \end{array} $	2. 668 2. 501 2. 378 2. 073 1. 927	100 9 5 36 6		
212 115 106 300 302	1. 869 1. 820 1. 785 1. 7449 1. 6684	5 7 11 39 10		
214	1. 6252	7		
116	1. 6075	19		
206	1. 5370	6		
220	1. 5112	9		
221	1. 4979	5		
304	1. 4877	27		
222	1. 4609	15		
117	1. 4334	3		
008	1. 4246	3		
312	1. 4071	1		
108	1. 3741	8		
216	1. 3701	3		
224	1. 3351	8		
314	1. 2940	3		
118	1. 2882	4		
225	1. 2595	4		
208	1. 2511	2		
404	1. 1895	2		
226	1. 1826	5		
322	1. 1752	2		

Lattice constants

		a	c
1960	Yakel, Koehler, Bertaut, and	6. 0428	11. 369
1962	Forrat. [1] National Bureau of Standards.	6. 0455	11. 394 at 25 °C.

 $<sup>^5</sup>$  The density based on pyenometer measurements of a pressed pellet is 7.5 g/cm $^3$  indicating the number of molecules per unit cell as 6.

The density of lutetium manganite calculated from the NBS lattice constants is 7.676 g/cm<sup>3</sup> at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal Standard, tungsten, a=3.1648 A		
	d	I	
218 316 410 411 412	A 1. 1561 1. 1534 1. 1425 1. 1370 1. 1203	5 5 5 2 1	
$\begin{array}{c} 1 \cdot 0 \cdot 10 \\ 227 \\ 308 \\ 406 \\ 1 \cdot 1 \cdot 10 \end{array}$	1. 1131 1. 1072 1. 1034 1. 0777 1. 0661	4 6 2 1 1	
$\begin{array}{ c c c }\hline & 414 \\ 2 \cdot 0 \cdot 10 \\ & 228 \\ & 502 \\ & 415 \\\hline \end{array}$	1. 0603 1. 0447 1. 0364 1. 0297 1. 0213	7 3 3 2 1	
$ \begin{array}{c} 318 \\ 1 \cdot 0 \cdot 11 \\ 330 \\ 332 \\ 2 \cdot 1 \cdot 10 \end{array} $	1. 0166 1. 0158 1. 0077 0. 9923 . 9874	4 1 4 2 2	
416 408 417 1.0.12 328	. 9791 . 9638 . 9351 . 9344 . 9181	4 1 2 1 3	
$3 \cdot 1 \cdot 10$ $2 \cdot 0 \cdot 12$	. 8964 . 8928	$\frac{3}{2}$	

#### Reference

[1] H. L. Yakel, W. C. Koehler, E. F. Bertaut, and E. F. Forrat, Erbium manganite—a new ABO<sub>3</sub> structure, Acta Cryst. **13**, 1015 (1960).

# Manganese(II) Tungstate (huebnerite), MnWO<sub>4</sub> (monoclinic)

#### Powder Data cards

Card number	Index lines	Radiation	Source
10-477	3. 00 2. 96 3. 78	Iron	Berry [1].

Additional published patterns. None.

NBS sample. The sample of manganese tung-state was prepared at NBS by reacting solutions of manganese (II) chloride and sodium tungstate. The precipitate was washed, dried, and heated to 1,000 °C for 10 min. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent of calcium.

The color of the sample was yellow brown. The refractive indices were not determined because the sample was too fine-grained.

The d-values of the three strongest lines are:

2.996, 2.954, and 4.84 A.

Structural data. Broch [2] in 1929 determined that manganese tungstate has magnesium tungstate structure, the space group  $C_{2n}^4$ —P2/c (No. 13), and 2(MnWO<sub>4</sub>) per unit cell. The lattice constants of Broch have been converted from kX to angstrom units for comparison with the NBS values.

The density of manganese tungstate calculated from the NBS lattice constants is 7.234 g/cm<sup>3</sup> at 25 °C.

#### References

[1] L. G. Berry, Queen's University, Kingston, Ontario, Canada.

	1962 Nation of Stan Cu, 1.5405 A	dards
hkl	Internal st tungsten, a=	andard,
	d	I
010 100	A 5. 76 4. 84	22 63
$011 \\ \frac{1}{1}0 \\ \overline{1}11$	3. 78 3. 70 2. 996	59 56 100
$ \begin{array}{c} 111 \\ 020 \\ 002, 021 \end{array} $	2. 954 2. 880 2. 497	95 29 54
120 200	2. 474 2. 416	9 19
$\begin{array}{c} \overline{1}02\\ \underline{1}21\\ \overline{1}12 \end{array}$	2. 237 2. 209 2. 087	$   \begin{array}{c}     16 \\     26 \\     7   \end{array} $
$\frac{112}{211}$	2. 057 2. 051	11 12
$egin{array}{c} 211 \\ 030 \\ 022 \\ \end{array}$	2. 021 1. 9205 1. 8871	$\begin{array}{c} 10 \\ 5 \\ 16 \end{array}$
220 130	1. 8507 1. 7843	16 26
$\begin{array}{c} \overline{1}22\\ \overline{2}02\\ \overline{2}21\end{array}$	1. 7666 1. 7539 1. 7440 1. 7266	$ \begin{array}{c}     6 \\     19 \\     19 \end{array} $
221 202	1. 7196	28 20
$\begin{array}{c} \overline{1}31 \\ \overline{2}12 \\ 131 \end{array}$	1. 6839 1. 6777 1. 6762	4 5 5
212 300	1. 6472 1. 6096	3 <b>3</b>
$013 \\ 310 \\ \overline{1}13$	1. 5996 1. 5501 1. 5273	$\begin{matrix} & 6 \\ 2 \\ 16 \end{matrix}$
032 113	1. 5221 1. 5100	12 12
$ \begin{array}{r}     230 \\     \hline{2}22 \\     \hline{3}11 \end{array} $	1. 5023 1. 4981 1. 4886	8 8 16
222 311	1. 4754 1. 4723	11 16
$     \begin{array}{r}                                     $	1. 4568 1. 4467 1. 4423	12 12 15
$\frac{320}{123}$	1. 4048 1. 3879	2 4
$\begin{array}{r} 041 \\ \underline{123} \\ \underline{3}02 \end{array}$	1. 3834 1. 3751 1. 3654	11 3 2
$     \begin{array}{r}                                     $	1. 3587 1. 3458	6 4
$ \begin{array}{r} 302 \\ \overline{141} \\ 141, \overline{3}12 \\ 213 \\ 312 \end{array} $	1. 3408 1. 3316 1. 3284 1. 3216 1. 3056	4 4 8 3 2
$\begin{array}{c} \overline{2}32\\ \overline{2}32\\ 232 \end{array}$	1. 2949 1. 2804	4 4

<sup>[2]</sup> E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norsk. Videns.-Akad. Oslo I. Mat.-Naturv. K1 1929, No. 8.

# Manganese (II) Tungstate (huebnerite), MnWO4 (monoclinic)—Continued

Lattice constants

	a	ь	с	β
1930 Broch [2]	A 4. 85 4. 829	A 5. 77 5. 759	A 4. 98 4. 998	90.88° 91.16° at 25 °C

# Mercury (II) Fluoride, HgF<sub>2</sub> (cubic)

Powder Data cards. None

Additional published patterns. None.

NBS sample. The sample of mercury (II) fluoride was obtained from the A. D. Mackay Company, Inc., New York, N.Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon, and 0.001 to 0.01 percent of tin.

The color of the sample was orange. The refractive index was not determined because of the small particle size.

The d-values of the three strongest lines are:

3.196, 1.9576, and 2.768 A.

Structural data. Ebert and Woitnek [1] in 1933 determined that mercury (II) fluoride has the fluorite structure, the space group O<sub>5</sub> —Fm3m (No. 225), and 4(HgF<sub>2</sub>) per unit cell. The lattice constant of Ebert and Woitnek has been converted from kX to angstrom units for comparison with the NBS value.

Lattice constants

1933 1962	Ebert and Woitnek [1] National Bureau of Standards_	A 5. 55 5. 5373 at 25 °C
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The density of mercury (II) fluoride calculated from the NBS lattice constant is 9.332 g/cm<sup>3</sup> at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standards, tungsten, $a=3.1648$ A		
	d	I	a
	A		A
111	3. 196	100	5. 536
200	2. 768	43	5. 537
220	1. 9576	46	5. 5369
311	1. 6695	40	5. 5371
222	1. 5983	8	5. 5367
400	1. 3844	7	5. 5376
331	1. 2705	12	5. 5380
420	1. 2383	9	5. 5378
422	1. 1302	9 <b>7</b>	5. 5368
511	1. 0657	7	5. 5375
440	0. 9789	4	5. 5377
531	. 9361	10	5. 5379
600	. 9229	7 8 8	5. 5373
620	. 8756	8	5. 5377
533	. 8444	8	5. 5368
622	. 8348	4	5. 5372
444	. 7993	2	5. 5374
Augrama	lue of last five l	inoa	5. 5373

#### Reference

[1] F. Ebert and H. Woitnek, Kristallstrukturen von Fluoriden. II. HgF, HgF<sub>2</sub>, CuF und CuF<sub>2</sub>, Z. anorg. u. allgem. Chem. **210**, 269–272 (1933).

#### Powder Data cards.

Card number	Index	Radiation	Source
1-1102	2. 55 4. 30 3. 58	Molybdenum	Dow Chemical Company, Midland, Michigan.

Additional published pattern. Hammel [1] 1939. NBS sample. The sample of nickel sulfate was prepared by heating nickel sulfate hexalydrate, obtained from Baker and Adamson Chemical Co., with H<sub>2</sub>SO<sub>4</sub> at 160 °C. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent each of aluminum, iron, magnesium, and silicon; and 0.0001 to 0.001 percent each of barium and copper.

The color of the sample was greenish-yellow. The optical sign and the  $N_{\beta}$  could not be determined because the sample was too fine-grained. The other refractive indices were  $N_{\alpha}=1.695$  and  $N_{\gamma}=1.723$ .

The d-values of the three strongest lines are:

2.553, 3.564, and 3.334 A.

Structural data. Dimaras [2] in 1957 determined the structure of nickel sulfate; it has the space group  $D_{2h}^{17}$ —Cmcm (No. 63) and 4(NiSO<sub>4</sub>) per unit cell. Hammel [1] had previously reported lattice constants for nickel sulfate as a = 4.63, b = 6.52, and c = 8.51 A.

Lattice constants

		a	. в	c
1957 1962	Dimaras [2] National Bureau of Standards.	A 5. 155 5. 1596	7. 842 7. 8362	A 6. 338 6. 3378 25 °C.

The density of nickel sulfate calculated from the NBS lattice constants is 4.011 g/cm<sup>3</sup> at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	I	
	A		
110	4. 314	41	
020	3. 921	28	
111	3. 564	80	
021	3. 334	50	
200	2. 579	47	
112 130 220 221 202	2. 553 2. 331 2. 156 2. 037 2. 001	$     \begin{array}{r}       100 \\       48 \\       3 \\       5 \\       27     \end{array} $	
040	1. 959	16	
132	1. 879	7	
023	1. 860	8	
222	1. 781	25	
310	1. 679	7	
042	1. 667	15	
311	1. 629	8	
004	1. 5845	10	
133	1. 5652	7	
241	1. 5147	7	
150	1. 4999	6	
312	1. 4839	12	
024	1. 4691	7	
151	1. 4592	3	
330	1. 4363	13	
242	1. 3996	26	
152	1. 3552	6	
134	1. 3104	5	
400	1. 2894	20	
243	1. 2545	3	
153	1. 2229	3	
115	1. 2161	4	
421	1. 2027	3	

# References

[1] F. Hammel, Contribution á l'étude des sulfates de la série magnésienne, Ann. chim. 11, 247–358 (1939).

[2] P. I. Dimaras, Morphology and structure of anhydrous nickel sulfate, Acta Cryst. 10, 313-315 (1957).

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of nickel tungstate was prepared at NBS by the reaction of solutions of nickel chloride and sodium tungstate. precipitate was washed, dried, and heated to 1,100 °C for 15 min. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of silicon; and 0.001 to 0.01 percent each of aluminum, calcium, lead, and magnesium.

The color of the sample was light brown. The refractive indices were not determined because

the sample was too fine-grained.

The  $\hat{d}$ -values of the three strongest lines are:

2.889, 1.6788, and 2.455 A.

Structural data. Broch [1] in 1929 determined that nickel tungstate has the magnesium tungstate structure, the space group  $C_{2h}^4$ —P2/c (No. 13), and 2 (NiWO<sub>4</sub>) per unit cell. The lattice constants of Broch have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

1930	Broch [1]	<i>a A</i> 4. 69	b A 5. 67	c A 4. 94	β 89. 67°
1957 1962	Keeling [2]. National Bureau of Standards.	4. 600	5. 66 5. 665	4. 91	90. 08° ≈ 90. at 25 °C

The density of nickel tungstate calculated from the NBS lattice constants is 7.952 g/cm<sup>3</sup> at 25 °C.

# References

- [1] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norsk. Videns.-Akad. Oslo I. Mat.-Naturv. Kl. **1929** No. 8.
- [2] R. O. Keeling, Jr., The structure of NiWO<sub>4</sub>, Acta Cryst. **10**, 209–213 (1957).

hkl (ortho.) <sup>6</sup>	1962 National Bureau of Standards Cu, 15405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
	d	I	
010 100 011 110 111	A 5. 67 4. 60 3. 71 3. 57 2. 889	$   \begin{array}{r}     7 \\     32 \\     34 \\     34 \\     100   \end{array} $	
020 002, 021 120 200 102, 121	2. 834 2. 455 2. 412 2. 301 2. 166	$   \begin{array}{c}     15 \\     39 \\     7 \\     12 \\     25   \end{array} $	
210 112 211 030 022	2. 131 2. 024 1. 955 1. 888 1. 856	$\begin{array}{c} 2\\11\\11\\3\\10\end{array}$	
220 130 122 202, 221 131	1. 786 1. 7471 1. 7208 1. 6788 1. 6452	$\begin{array}{c} 7 \\ 19 \\ 6 \\ 40 \\ 1 \end{array}$	
212 013 300 032 113	1. 6091 1. 5729 1. 5337 1. 4973 1. 4882	$\begin{array}{c} 2\\ 3\\ 2\\ 4\\ 17 \end{array}$	
$ \begin{array}{c c} 310 \\ 230 \\ 222 \\ 132 \\ 311,023 \end{array} $	1. 4801 1. 4596 1. 4441 1. 4234 1. 4173	$\begin{array}{c} 2\\ 3\\ 7\\ 16\\ 23 \end{array}$	
$\begin{bmatrix} 041\\ 123\\ 320\\ 141\\ 302, 321 \end{bmatrix}$	1. 3609 1. 3546 1. 3485 1. 3047 1. 3008	7 3 1 5 7	
312 232 004, 042 223, 240 330	1. 2676 1. 2549 1. 2276 1. 2068 1. 1905	3 3 3 3 5	
322 241 114 400 050	1. 1824 1. 1712 1. 1610 1. 1498 1. 1331	$\begin{array}{c} 2 \\ 7 \\ 1 \\ 2 \\ 1 \end{array}$	
410, 024 150 411, 313	1. 1266 1. 0998 1. 0980	1 4 7	

<sup>6 (</sup>Separation of monoclinic doublets was not detected in the NBS pattern, so it was indexed as orthorhombic.)

# Potassium Chlororhenate, K<sub>2</sub>ReCl<sub>6</sub> (cubic)

# Powder Data cards

Card number	Index lines	Radiation	Source
3-0085	5. 7 2. 47 2. 98	Copper	Aminoff [1] 1936.

Additional published patterns. None.

NBS sample. The sample of potassium chlor-orhenate was prepared at NBS by R. Johannesen from chlororhenic acid. Spectrographic analysis showed the following impurities: 0.001 to 0.01 percent silicon, sodium, and rubidium; and 0.0001 to 0.001 percent of calcium.

The color of the sample was yellow. The refractive index could not be determined because the

color was too intense.

The *d*-values of the three strongest lines are:

5.68, 3.48, and 2.967 A.

Structural data. Aminoff [1] in 1936 determined that potassium chlororhenate has the potassium chloroplatinate structure, the space group  $O_h^5$ —Fm3m (No. 225) and  $4(K_2ReCl_6)$  per unit cell. The unit cell measurement reported by Aminoff has been converted from kX to angstrom units for comparison with the NBS value.

#### Lattice constants

1936 Aminoff [1]	9. 881
1962 National Bureau of Stand-	9. 840 at
ards.	25 °C.

The density of potassium chlororhenate calculated from the NBS lattice constant is 3.325 g/cm<sup>3</sup> at 25 °C.

#### Reference

Brita Aminoff, Über die Kristallstruktur von K<sub>2</sub>ReCl<sub>6</sub>,
 Krist. (A) 94, 246-248 (1936).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, silver, a=4.0861 A		
	d	I	a
111 200 220 311 222	A 5. 68 4. 92 3. 48 2. 967 2. 840	100 39 42 42 8	A 9. 84 9. 85 9. 84 9. 842 9. 839
400 331 420 422 511	2. 460 2. 257 2. 201 2. 008 1. 894	40 15 15 15 15	9. 841 9. 838 9. 843 9. 840 9. 842
440 531 600 620 533	1. 739 1. 663 1. 640 1. 556 1. 500	19 13 6 4 3	9. 840 9. 839 9. 839 9. 838 9. 839
$444 \\ 711 \\ 640 \\ 642 \\ 731$	1. 420 1. 3781 1. 3647 1. 3152 1. 2813	5 6 2 4 3	9. 840 9. 842 9. 841 9. 842 9. 842
800 733 820 822 751	1. 2300 1. 2022 1. 1933 1. 1598 1. 1364	$ \begin{array}{c c} <1\\ <1\\ 2\\ 2\\ \end{array} $	9. 840 9. 840 9. 840 9. 841 9. 842
840 911 842 664 931	1. 1003 1. 0803 1. 0740 1. 0491 1. 0315	$\begin{array}{c c} & 3 & \\ & 2 & \\ & 2 & \\ < 1 & \\ < 1 & \end{array}$	9. 841 9. 842 9. 843 9. 841 9. 840
$\begin{array}{c} 844 \\ 933 \\ 10.0.0 \\ 10.2.0 \\ 951 \end{array}$	1. 0046 0. 9890 . 9843 . 9650 . 9514	$\begin{array}{c c} & 2 \\ & 1 \\ < 1 \\ & < 1 \end{array}$	9. 843 9. 840 9. 843 9. 841 9. 841
$\begin{array}{c} 953 \\ 10.4.0 \\ 10.4.2 \\ 11.1.1 \\ 880 \end{array}$	. 9175 . 9135 . 8984 . 8874 . 8699	$\begin{array}{c c} & 1 \\ & 2 \\ & \leq 1 \\ & \leq 1 \end{array}$	9. 839 9. 839 9. 841 9. 842 9. 842
$11 \cdot 3 \cdot 1$ $10 \cdot 4 \cdot 4$ $10 \cdot 6 \cdot 0$ $11 \cdot 3 \cdot 3$ $12 \cdot 0 \cdot 0$	. 8598 . 8567 . 8439 . 8347 . 8201	$\begin{array}{c c} & 3 \\ < 1 \\ < 1 \\ < 1 \\ 1 \end{array}$	9. 841 9. 843 9. 841 9. 841 9. 841
11.5.1 $12.2.2$ $11.5.3$	. 8115 . 7981 . 7904	$\begin{cases} 1 \\ \leq 1 \\ 1 \end{cases}$	9. 839 9. 840 9. 840
Average va	Average value of last five lines		

# Potassium Nitroso Chlororuthenate, K<sub>2</sub>RuCl<sub>5</sub>NO

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of potassium nitroso chlororuthenate was prepared at NBS by R. Johannesen by heating together on a steam bath a soluble ruthenium salt, potassium chloride, and concentrated nitric acid.

The color of the sample was very dark red. The refractive indices are  $N_{\alpha}=1.750$ ,  $N_{\beta}=1.762$ , and  $N_{\gamma}=1.777$ . 2V is approximately 90°. The d-values of the three strongest lines are: 5.75, 5.62, and 2.594 A.

Structural data. The structure of potassium

nitroso chlororuthenate has not been reported.

1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A		
d	I	
A 6. 50 6. 39 6. 13 5. 75 5. 62	$     \begin{array}{c}                                     $	
5. 28 5. 20 4. 79 4. 36 4. 08	$ \begin{array}{c c} 17 \\ 27 \\ 29 \\ < 4 \\ 6 \end{array} $	
3. 96 3. 73 3. 52 3. 45 3. 328	10 4 23 27 16	
3. 176 3. 091 3. 059 3. 027 2. 996	$ \begin{array}{c c}  & <4 \\  & 12 \\  & 11 \\  & 15 \\  & 14 \end{array} $	
2. 934 2. 873 2. 805 2. 720 2. 632	7 13 36 36 36 8	
2. 594 2. 481 2. 409 2. 393 2. 277	$ \begin{array}{c c} 48 \\ < 4 \\ 7 \\ 10 \\ 15 \end{array} $	
2. 262 2. 211 2. 167 2. 137 2. 105	$ \begin{array}{c c} 10 \\ 10 \\ < 4 \\ < 4 \\ 7 \end{array} $	
2. 071 2. 063 2. 037 1. 999 1. 980	14 16 7 4 10	

# Rubidium Perchlorate, RbClO<sub>4</sub> (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium perchlorate was prepared at NBS by the reaction of a solution of rubidium nitrate with perchloric acid. The precipitate was recrystallized several times to improve the purity. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of cesium, potassium, and sodium; and 0.001 to 0.01 percent of silicon.

The sample is colorless and optically negative with the indices of refraction  $N_{\alpha}=1.465$ ,  $N_{\beta}=$ 

1.470, and  $N_{\gamma} = 1.472$ .  $2V = 60^{\circ}$ .

The d-values of the three strongest lines are:

3.63, 3.26, and 2.228 A.

Structural data. Büssem and Herrmann [1] in 1928 determined that rubidium perchlorate has the potassium sulfate structure, the space group D<sub>2h</sub>-Pbnm (No. 62), and 4(RbClO<sub>4</sub>) per unit cell. At 279 °C the orthorhombic form transforms to face-centered cubic. The lattice constants of Büssem and Herrmann have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	b	c
1928	Büssem and	A $7.55$	$\begin{array}{c c} A \\ 9.29 \end{array}$	A 5. 82
1962	Herrmann [1]. National Bureau of Standards	7. 490	9. 269	5. 814 at
	of Standards.			25 °C

The density of rubidium perchlorate calculated from the NBS lattice constants is 3.042 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] W. Büssem and K. Herrmann, Röntgenographische Untersuchung der einwertigen Perchlorate, Z. Krist 67, 405–408 (1928).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A	
	d	I
111 200 021 210 121	A 4. 12 3. 74 3. 63 3. 47 3. 26	23 41 100 50 89
211 002 130 221 022	2. 982 2. 907 2. 858 2. 605 2. 464	51 37 7 22 8
310 230 122 040 311	2. 410 2. 384 2. 339 2. 318 2. 228	$\begin{array}{c} 3 \\ 4 \\ 16 \\ < 1 \\ 60 \end{array}$
140 231 041 321 132	2. 214 2. 206 2. 153 2. 057 2. 038	38 38 8 <1 4
330 103 400 331 410	1. 9418 1. 8765 1. 8725 1. 8416 1. 8356	10 3 3 5 4
150 023 142 411 123	1. 7997 1. 7875 1. 7609 1. 7505 1. 7387	$egin{array}{c} 1 \\ 5 \\ 10 \\ 4 \\ 6 \end{array}$
420 340 213 421 250	1. 7357 1. 6984 1. 6928 1. 6633 1. 6609	$\begin{array}{c}4\\4\\8\\1\\2\end{array}$
332 251 402 412 431	1. 6145 1. 5970 1. 5741 1. 5518 1. 5438	13 3 2 5 2
303	1. 5303	1

## Rubidium Periodate, RbIO<sub>4</sub> (tetragonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of rubidium periodate was prepared at NBS by the reaction of solutions of sodium periodate and rubidium nitrate. The precipitate obtained was recrystallized several times to improve the purity. Spectrographic analysis showed the following impurities: 0.1 to 1.0 percent of sodium; 0.01 to 0.1 percent of potassium; and 0.001 to 0.01 percent each of cesium and silicon.

The sample was colorless and optically positive with the refractive indices  $N_o$ =1.603 and  $N_e$ =

1.621.

The d-values of the three strongest lines are:

3.52, 2.193, and 2.961 A.

Structural data. Beintema [1] in 1937 determined that rubidium periodate has the scheelite structure, the space group C<sub>4h</sub><sup>6</sup>—I4<sub>1</sub>/a (No. 88), and 4(RbIO<sub>4</sub>) per unit cell. The unit cell measurements reported by Beintema have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
1937 1962	Beinteina [1] National Bureau of of Standards.	A 5. 89 5. 921	A 12. 96 13. 052 at 25 °C.

The density of rubidium periodate calculated from the NBS lattice constants is 4.011 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] J. Beintema, Die Kristallstruktur der Alkaliperrhenate und—jodate, Z. Krist **97A**, 300–332 (1937).

hkl	of Sta Cu, 1.5405 Internal	onal Bureau andards of A at 25 °C standard, $a=3.1648$ A
	d	I
101 112 004 200 202	A 5. 39 3. 52 3. 26 2. 961 2. 694	$ \begin{array}{c} 14 \\ 100 \\ 17 \\ 20 \\ < 1 \end{array} $
211 114 213 204 220	2. 594 2. 573 2. 262 2. 193 2. 093	$\begin{array}{c} 3 \\ 2 \\ 1 \\ 22 \\ 10 \end{array}$
222 116 215 312 224	1. 9939 1. 9301 1. 8585 1. 7994 1. 7618	
321, 008 305 323 217 400	1. 6300 1. 5739 1. 5356 1. 5237 1. 4796	$egin{pmatrix} 2\\ < 1\\ < 1\\ 2 \end{pmatrix}$
208 316 332 404 420	1. 4283 1. 4186 1. 3642 1. 3476 1. 3237	6 9 4 3 3
$ \begin{array}{r} 228 \\ 1 \cdot 1 \cdot 10 \\ 424 \\ 501 \\ 336 \end{array} $	1. 2864 1. 2454 1. 2262 1. 1788 1. 1750	${ \begin{array}{c} 2 \\ 1 \\ 3 \\ < 1 \\ 1 \end{array} }$
512 408 0.0·12 3·1·10 440	1. 1438 1. 0964 1. 0880 1. 0711 1. 0468	3 1 <1 1 <1
428 516 2.0.12 532 444	1. 0283 1. 0248 1. 0212 1. 0034 0. 9969	$egin{array}{c} 1 \\ 2 \\ 1 \\ 1 \\ 1 \\ 1 \end{array}$
$\begin{array}{c} 600 \\ 2 \cdot 2 \cdot 12 \\ 3 \cdot 3 \cdot 10 \\ 604 \\ 620 \end{array}$	. 9869 . 9650 . 9532 . 9447 . 9363	<1 1 <1 <1 <1
536 1·1·14 624 448	. 9200 . 9100 . 8997 . 8808	<1 1 3

## Silver Selenate, Ag<sub>2</sub>SeO<sub>4</sub> (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of silver selenate was obtained from City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following major impurities: 0.1 to 1.0 percent sodium; and 0.001 to 0.01 percent each of calcium, magnesium, and silicon.

The color of the sample was grey-white. The indices of refraction could not be determined because the sample was too fine-grained.

The d-values of the three strongest lines are:

2.930, 2.742, and 3.246 A.

Structural data. Herrman and Ilge [1] in 1931 determined that silver selenate has the silver sulfate structure, the space group D<sub>2h</sub><sup>24</sup>—Fddd (No. 70), and 8(Ag<sub>2</sub>SeO<sub>4</sub>) per unit cell. The unit cell measurements reported by Herrman and Ilge have been converted from kX to angstrom units for comparison with the NBS values.

Lattice constants

	a	b	c
1931 Herrman and Ilge [1]. 1962 National Bu- reau of Standards.	10. 388	A 12. 841 12. 981	A 6. 081 6. 0499 at 25 °C

The density of silver selenate calculated from the NBS lattice constants is 5.839 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] K. Herrman and W. Ilge, Die Struktur des Silbersulfats, Z. Krist. 80, 402–415 (1931).

	1	
hkl	1962 Nation of Stan Cu, 1.5405 A Internal st tungsten, a=	dards A at 25 °C andard,
	d	· I
220 040 311 022 202	A 4. 061 3. 246 2. 930 2. 742 2. 615	6 73 100 81 4
331	2. 469	37
222	2. 425	4
151	2. 325	3
242	2. 036	4
260	1. 997	4
351	1. 965	37
511	1. 945	6
531	1. 791	2
062	1. 7599	23
313	1. 7278	15
620	1. 6740	7
080	1. 6226	6
333	1. 6170	14
371	1. 5786	12
004	1. 5127	7
602	1. 5038	7
353	1. 4473	6
224	1. 4173	<1
044	1. 3707	8
642	1. 3638	10
660	1. 3523	7
391	1. 3001	5
373	1. 2698	4
751	1. 2610	1
0·10·2	1. 1926	5
315	1. 1380	3
911	1. 1303	2
624	1. 1222	3
393	1. 1110	2
084	1. 1064	3
682 3·11·1 0·12·0 355,862 6·10·0	1. 1033 1. 0985 1. 0817 1. 0456 1. 0391	3 2 2 2 2 3
664	1. 0083	2
026	0. 9966	1
3·11·3	. 9771	1

## Sodium Cyanate, NaCNO (trigonal)

Powder Data cards. None.

Additional published pattern. None.

NBS sample. The sample of sodium cyanate was obtained from the City Chemical Corp., New York, N.Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, iron, magnesium, and silicon; and 0.001 to 0.01 percent each of barium, nickel,

The color of the sample was white and it is optically positive. The indices of refraction are  $N_e=1.629$ , and  $N_o\approx 1.390$  The d-values of the three strongest lines are:

2.872, 1.794, and 2.167 A.

Structural data. Bassière [1] in 1938 determined that sodium cyanate has the sodium hydrofluoride structure, the space group  $C_{3v}^{5}$ —R3m (No. 160) with 3(NaCNO) per unit cell. The unit cell measurements reported by Bassière have been coverted from kX to angstrom units for comparison with the NBS values.

Lattice constants

		a	c
1938 1962	Bassière [1] National Bureau of Standards.	A 3. 583 3. 5851	A 15. 13 15.110 at 25 °C.

The density of sodium cyanate calculated from the NBS lattice constants is 1.949 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] M. Bassière, Sur la structure de l'isocyanate de sodium, Compt. rend. 206, 1309-1311 (1938)

## Sodium Orthotungstate (VI) Dihydrate, Na<sub>2</sub>WO<sub>4</sub> • 2H<sub>2</sub>O (orthorhombic)

#### Powder Data cards

	ard nber	Index	Radiation	Source
1-0	0107	6. 9 4. 22 3. 17	Molybdenum	Hanawalt, Rinn, and Frevel [1] 1938.

Additional published patterns. None.

NBS sample. The sample of sodium orthotungstate dihydrate was obtained from the Allied Chemical and Dye Corp., New York, N.Y. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent silicon, and 0.001 to 0.01 percent each of calcium and lead.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A	
	d	I
003 101 012 006 104	$\begin{matrix} A \\ 5.038 \\ 3.044 \\ 2.872 \\ 2.517 \\ 2.400 \end{matrix}$	7 11 100 1 10
015 110 107 113 009	2. 167 1. 794 1. 774 1. 689 1. 6788	18 21 9 2 2
018 021 202 116 024	1. 6134 1. 5442 1. 5210 1. 4605 1. 4357	$ \begin{array}{c c} 2 \\ < 1 \\ 6 \\ < 1 \\ 1 \end{array} $
$ \begin{array}{c c} 205 \\ 1.0.10 \\ 027 \\ 119 \\ 208 \end{array} $	1. 3810 1. 3589 1. 2600 1. 2253 1. 1989	$\begin{bmatrix} 2 \\ 3 \\ 3 \\ 1 \\ < 1 \end{bmatrix}$
$ \begin{array}{c c} 122 \\ 214 \\ 125 \\ 0.2.10 \\ 300 \end{array} $	1. 1595 1. 1206 1. 0937 1. 0827 1. 0348	$\begin{array}{c c} 2\\1\\ < 1\\1\\1\end{array}$
$\begin{array}{c} 217 \\ 0.1.14 \\ 2.1.10 \\ 1.0.16 \\ 220 \end{array}$	1. 0307 1. 0194 0. 9270 . 9035 . 8964	$\begin{pmatrix} 2 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$
2.0.14	. 8863	<1

The sample is colorless and optically positive. The indices of refraction are  $N_{\alpha}=1.554$ ,  $N_{\beta}=1.556$ , and  $N_{\gamma}=1.568$ .

The *d*-values of the three strongest lines are:

6.91, 3.17, and 4.23 A.

Lattice constants

		a	b	c
1960 1962	Pistorius [3] National Bu- reau of Standards.	A 10. 601 10. 604	A 13. 842 13. 844	A 8. 456 8. 455 at 25 °C.

The density of sodium orthotungstate dihydrate calculated from the NBS lattice constants is 3.523 g/cm<sup>3</sup> at 25 °C.

# Sodium Orthotungstate(VI) Dihydrate, Na<sub>2</sub>WO<sub>4</sub>·2H<sub>2</sub>O (orthorhombic)—Con.

Structural data. Poljak and Becka [2] in 1958 determined that sodium orthotungstate dihydrate is isomorphous with sodium orthomolybdate dihydrate, having the space group  $D_{2h}^{15}$ —Pbca (No. 61) and  $8(Na_2WO_4\cdot 2H_2O)$  per unit cell.

		<del></del>
hkt	1962 Nation of Star Cu, 1.5405 Internal silver, $a=$	dards A at 25 °C tandard,
	d	I
020 111 200 121 002	A 6. 91 5. 98 5. 29 4. 78 4. 23	100 22 21 15 63
220 131 022 040 122	4. 21 3. 79 3. 61 3. 46 3. 42	2 15 60 17 6
202 231 311 141 132	3. 309 3. 221 3. 173 3. 069 2. 988	47 14 80 36 54
$240 \\ 241 \\ 232 \\ 331, 312 \\ 410$	2. 898 2. 745 2. 684 2. 664 2. 601	22 6 43 38 6
151 420 250 242 251	2. 556 2. 475 2. 457 2. 394 2. 359	1 2 6 11 8
133 060 430 043, 161 143	2. 347 2. 309 2. 302 2. 181 2. 145	8 6 6 30 8
$\begin{array}{c} 252 \\ 004, 351 \\ 440 \\ 511 \\ 062 \end{array}$	2. 121 2. 112 2. 106 2. 034 2. 028	15 12 4 30 20
$   \begin{array}{c}     162 \\     521 \\     450 \\     171 \\     442   \end{array} $	1. 993 1. 970 1. 915 1. 894 1. 886	18 6 3 22 12
531 270 271 063 433	1. 879 1. 855 1. 809 1. 789 1. 784	15 4 6 6 5
$600 \\ 172 \\ 452$	1. 766 1. 764 1. 746	8 9 8

hkl	1962 Nation of Stan Cu, 1.5405 A Internal stailver, a=	dards A at 25 °C tandard,		
	d	I		
080 353	A 1. 732 1. 728	$\begin{array}{c} 2\\11\end{array}$		
620	1. 712	9		
272	1. 699	5		
513	1. 684	19		
621, 181	1. 676	19		
551	1. 652	7		
523	1. 646	5		
462	1. 610	3		
344	1. 605	6		
372	1. 596	9		
363	1. 592	9		
182	1. 583	5		
640	1. 576	4		
552	1. 563	4		
064	1. 559	3		
632	1. 538	1		
561	1. 535	1		
282	1. 531	3		
235	1. 521	7		
145	1. 508	2		
191	1. 500	2		
650	1. 489	3		
472	1. 486	10		
711	1. 483	8		
642	1. 476	2		
623	1. 464	7		
291, 480, 335 553 174, 155 364, 702	1. 452 1. 445 1. 431 1. 426	2 3 1 2		
534, 283	1. 422	5		
415	1. 418	5		
652	1. 405	2		
660	1. 402	2		
345	1. 396	3		
0·10·0	1. 386	2		
643, 544	1. 373	2		
563	1. 365	2		
604	1. 356	10		

#### References

J. D. Hanawalt, H. W. Rinn, and L. K. Frevel, Chemical analysis by X-ray diffraction, Ind. Eng. Chem. Anal. Ed. 10, 457-512 (1938).
 R. J. Poljak and L. N. Becka, Estudio cristalográfico del molbdato de sodio dihidrato, Anales asoc. quím. argentina, 46, 199-203 (1958).
 C. W. F. T. Pistorius, Unit cell and space group of sodium molybdate dihydrate, Z. Krist. 114, 154-155 (1960).

## Sodium Tetrametaphosphate Tetrahydrate, high form Na<sub>4</sub>P<sub>4</sub>O<sub>12</sub>·4H<sub>2</sub>O (triclinic)

#### Powder Data cards

Card number	Index lines	Radiation	Source
*11-389	9. 4 5. 2 3. 10	Copper	Corbridge and Tromans (1) 1958.

<sup>\*</sup>This card refers to the high form and identifies it as alpha-sodium tetra-metaphosphate tetrahydrate.

Additional published patterns. Thilo and Rätz [2] 1949, Bell, Audrieth, and Hill [3] 1952, and

Bonneman [4] 1937.

NBS sample. The sample of sodium tetrametaphosphate tetrahydrate was prepared at NBS by H. Ondik according to the Warschauer [5] process and purified by the method used by Barney and Gryder [6]. The triclinic form was obtained by precipitating very slowly from solutions with alcohol above approximately 30 °C. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, chromium, and tungsten; and 0.001 to 0.01 percent each of iron, magnesium, manganese, nickel, silver, tin, titanium, and zirconium.

The sample is colorless.

The d-values of the three strongest lines are:

5.17, 9.25, and 3.075 A.

Structural data. Ondik [7] in 1961 determined the structure of the high temperature form of sodium tetrametaphosphate tetrahydrate which has the space group  $C_i^1$ — $P\bar{1}$  (No. 2) with 1 (Na<sub>4</sub>P<sub>4</sub>O<sub>12</sub>·4H<sub>2</sub>O) per unit cell. The low temperature form of sodium tetrametaphosphate tetrahydrate is reported on Powder Data cards numbered 11–15 and 11–15a.

The density of sodium tetrametaphosphate tetrahydrate calculated from the NBS lattice

constants is 2.146 g/cm<sup>3</sup> at 25 °C.

#### References

[1] D. E. C. Corbridge and F. R. Tromans, Identification of sodium phosphates with an x-ray focusing camera, Anal. Chem. 30, 1101-1110 (1958).

[2] E. Thilo and R. Rätz, Über die Kionstituten des Natriumtetraphosphates und Eigenschaften der Tetraphosphate, Z. anorg. Chem. 260, 255–266 (1949).

[3] R. N. Bell, L. F. Audrieth, and O. F. Hill, Preparation of sodium tetrametaphosphate, Ind. Eng. Chem. 44, No. 3, 568-572 (1952).

[4] P. Bonneman, Sur les tétramétaphosphates, Compt. rend. 204, 865 (1937).

[5] F. Warschauer, Z. anorg. allgem. Chem. 36, 137 (1903).
[6] D. L. Barney and J. W. Gryder, An ion-exchange purification of sodium tetrametaphosphate. J. Am.

purification of sodium tetrametaphosphate, J. Am. Chem. Soc. 77, 3195–3198 (1955).

[7] Helen M. Ondik and Stanley Block, The structure of the monoclinic form of sodium tetrametaphosphate tetrahydrate, Acta Cryst. 14, 555–561 (1961).

hkl	1962 Nation of Stan Cu, 1.5405 A Internal S Tungsten, a=	dards A at 25 °C tandard,
	d	I
$\begin{array}{c} 010 \\ 100 \\ 001 \\ 0\overline{1}1 \\ \overline{1}10 \\ \end{array}$	$A \\ 9.25 \\ 6.31 \\ 5.83 \\ 5.64 \\ 5.56$	95 31 30 54 9
101 110 111 020 011	5. 17 4. 90 4. 756 4. 616 4. 438	100 65 30 8 25
$ \begin{array}{c c} \hline 111 \\ \hline 120 \\ 1\overline{1}1 \\ 120 \\ 1\overline{2}1 \\ 021 \end{array} $	4. 300 3. 988 3. 803 3. 505 3. 332 3. 234	34 13 46 30 39 67
$\begin{bmatrix} \frac{021}{201} \\ 200 \\ \frac{210}{112,030} \\ 031 \end{bmatrix}$	3. 227 3. 153 3. 115 3. 075	37 24 91 93
$ \begin{array}{c c}     \hline     \hline   $	3. 046 3. 037 2. 920 2. 867 2. 819	32 32 12 3 28
$\begin{array}{c} \overline{13}1\\ \overline{2}20\\ \overline{1}12\\ \overline{22}1\\ \overline{2}21\end{array}$	2. 795 2. 785 2. 724 2. 656 2. 637	$\begin{array}{c} 35 \\ 11 \\ 5 \\ 23 \\ 24 \end{array}$
130 121 012 131 031	2. 631 2. 609 2. 598 2. 514 2. 471	$\begin{array}{c} 30 \\ 41 \\ 38 \\ 8 \\ 21 \end{array}$
$ \begin{array}{c c} 0\overline{3}2 \\ 220 \\ \overline{13}2 \\ 1\overline{2}2 \\ 102 \end{array} $	2. 461 2. 454 2. 428 2. 385 2. 378	42 34 1 8 18
$ \begin{array}{c c}     \hline     \hline   $	2. 367 2. 326 2. 309 2. 268 2. 235	14 7 5 8 7
$ \begin{array}{c c} 1\overline{4}1, \overline{2}31 \\ 1\overline{4}1 \\ 1\overline{3}2 \\ \overline{3}11 \\ \overline{2}22 \end{array} $	2. 220 2. 209 2. 180 2. 172 2. 148	$\begin{array}{c} 13 \\ 21 \\ 7 \\ 7 \\ 1 \end{array}$
$ \begin{array}{r}     \hline     310 \\     \hline     113 \\     300 \\     \hline     230 \\     \hline     142, 123 \end{array} $	2. 112 2. 106 2. 102 2. 067 2. 054	13 15 11 5 7

## Sodium Tetrametaphosphate Tetrahydrate, high form Na<sub>4</sub>P<sub>4</sub>O<sub>13</sub>·4H<sub>2</sub>O (triclinic)—Con.

Lattice constants

		a	ь	c	α	β	γ
1962	National Bureau o Standards.	$\begin{array}{c c} A \\ 6.655 \end{array}$	$\begin{array}{c c} A \\ 9.577 \end{array}$	A 6. 321	103. 40°	106. 98°	93. 29° at 25 °C

## Strontium Arsenate, Sr<sub>3</sub>(AsO<sub>4</sub>)<sub>2</sub> (trigonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of strontium arsenate was prepared at NBS by reacting solutions of strontium chloride and arsenic(V) acid. The precipitate was washed several times, dissolved in nitric acid, reprecipitated by addition of ammonia, and heated to 1,110 °C for 1 hour. Speetrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, antimony, lead, and silicon; and 0.001 to 0.1 percent each of barium, calcium, eopper, iron, magnesium, and tin.

The sample was eolorless and too fine-grained to allow determination of the indices of refraction.

The d-values of the three strongest lines are:

3.08, 2.796, and 2.071 A.

Structural data. Durif [1] in 1959 determined that strontium arsenate is isostructural with strontium phosphate, with the space group  $D_{3d}^5 - R_{3m}$  (No. 166) and  $1[Sr_3(AsO_4)_2]$  per rhombohedral unit cell or  $3[Sr_3(AsO_4)_2]$  per hexagonal unit cell.

Lattice constants

		a	c
1959 1962	Durif [1] National Bureau of Standards.	A 5. 581 5. 587	A 19.98 20.004 at 25 °C

The density of strontium arsenate ealeulated from the NBS lattiee eonstants is 4.980 g/em<sup>3</sup> at 25 °C.

#### Reference

[1] A. Durif, Structure cristalline des orthovanadates et orthoarseniates de baryum et de strontium, Acta Cryst. 12, 420-421 (1959).

hkl (hex.)	of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A					
	d	<i>I</i>				
006 015 110 202 009	A 3. 33 3. 08 2. 796 2. 352 2. 223	3 100 96 8 9				
024 205 1.0.10 119, 208 125	2. 178 2. 071 1. 8489 1. 7394 1. 6639	6 50 33 2 34				
$ \begin{array}{c c} 300 \\ 0.2.10 \\ 2.0.11 \\ 220 \\ 2.1.10 \\ 0.0.15 \end{array} $	1. 6129 1. 5421 1. 4537 1. 3970 1. 3502	19 13 2 17 18				
$\begin{array}{c} 0.0.15 \\ 315 \\ 1.1.15 \\ 229, 318 \\ 045 \\ \end{array}$	1. 3338 1. 2725 1. 2036 1. 1826 1. 1579	2 13 12 2 6				
1.2.14 1.3.10 235 410 4.0.10, 327	1. 1259 1. 1148 1. 0695 1. 0558 1. 0351	<1 10 8 8 4				
$ \begin{array}{c} 3.0.15 \\ 1.3.13 \\ 0.1.20 \\ 3.2.10 \\ 2.2.15 \end{array} $	1, 0278 1, 0116 0, 9795 . 9706 . 9646					
$ \begin{array}{c} 419 \\ 505 \\ 330 \\ 2.0.20 \\ 2.1.19 \end{array} $	. 9538 . 9405 . 9312 . 9244 . 9125					
425 1·2·20 0·5·10, 247	. 8913 . 8775 . 8711	6 5 3				
$2.4.10,\ 517$	. 8315	5 5				
$\begin{array}{ c c c c }\hline & 4.1.15 \\ & 4.2.11 \\ & 600 \\ & 3.1.20 \\ & 1.1.24 \\ \hline \end{array}$	. 8278 . 8169 . 8063 . 8019 . 7987	$ \begin{array}{c} 12 \\ < 1 \\ 4 \\ 4 \\ 2 \end{array} $				
$ \begin{array}{r} 5.1.10 \\ 1.0.25 \\ 345 \end{array} $	. 7969 . 7894 . 7801	5 2 5				

## Thallium (I) Arsenate, Tl<sub>3</sub>AsO<sub>4</sub> (hexagonal)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of thallous arsenate was prepared at NBS by reaction of a solution of thallous sulfate with a solution of arsenic oxide in concentrated nitric acid. The sparingly soluble precipitate was recrystallized from a boiling aqueous solution. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent each of aluminum, calcium, silicon, and sodium; and 0.001 to 0.01 percent each of copper, iron, lead, and magnesium.

The sample was pale yellow. The indices of refraction were not determined because they

were greater than 2.00.

The d-values of the three strongest lines are:

3.015, 3.303, and 2.786 A.

Structural data. No reference was found for the structure of thallous arsenate; however, it is thought to be isostructural with thallous phosphate, with the space group  $C_6^6 - P6_3$  (No. 173) and  $2(Tl_3AsO_4)$  per unit cell.

Lattice constant

		a	c
1962	National Bureau of Standards.	A 8. 516	5.234 at 25° C.

The density of thallous arsenate calculated from the NBS lattice constants is 7.596 g/cm<sup>3</sup> at 25 °C. The average density obtained with the Berman balance was 7.51 g/cm<sup>3</sup> at 25 °C.

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, $a=3.1648$ A				
	d	I			
100 110 200 111 201	A 7. 39 4. 26 3. 687 3. 303 3. 015	8 30 26 97 100			
210 002 300 112 301	2. 786 2. 617 2. 458 2. 230 2. 226	58 25 19 11 11			
202 220 310 221 212	2. 135 2. 130 2. 0451 1. 9721 1. 9076	11 9 24 6 46			
311 400 302 320 222	1. 9053 1. 8437 1. 7924 1. 6920 1. 6518	49 3 7 5 3			
312 203 411 402 213	1. 6113 1. 5778 1. 5384 1. 5074 1. 4788	$\begin{array}{c} 40 \\ 16 \\ 4 \\ 1 \\ < 1 \end{array}$			
500 322, 501 420 331 223	1. 4752 1. 4202 1. 3937 1. 3702 1. 3500	$\begin{array}{c} 3 \\ 12 \\ 5 \\ 2 \\ 1 \end{array}$			
421 313 004 502 114	1. 3471 1. 3276 1. 3091 1. 2851 1. 2511	$\begin{array}{c} 1 \\ 7 \\ 4 \\ 6 \\ 1 \end{array}$			
422 323 601 431, 520 304	1. 2303 1. 2147 1. 1965 1. 1811 1. 1551	$ \begin{array}{cccccccccccccccccccccccccccccccccccc$			
503 314 333 423 522	1. 1264 1. 1023 1. 1010 1. 0893 1. 0764	6 3 4 1 5			

## Thallium(I) Perchlorate, TlClO<sub>4</sub> (orthorhombic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of thallium perchlorate was prepared at NBS by reaction of solutions of thallium(I) sulfate and barium perchlorate. The product was purified by recrystallization. Spectrographic analysis showed the following to be the chief impurity: 0.001 to 0.01 percent

The sample was colorless and optically negative with the refractive indices  $N_{\alpha}=1.640$ ,  $N_{\beta}=1.644$ ,

 $N_{\gamma}$ =1.647, and 2V  $\simeq$  70°. The *d*-values of the three strongest lines are:

3.64, 2.234, and 3.278 A.

Structural data. Büssem and Herrmann [1] in 1928 determined that thallium(I) perchlorate has the BaSO<sub>4</sub> structure, the space group D<sub>2h</sub><sup>16</sup>-Pbnm (No. 62), and 4(TlClO<sub>4</sub>) per unit cell. According to Herrmann and Ilge [2] and Braekken and Harang [3], at temperatures above 266 °C, there exists a cubic form with the KClO<sub>4</sub> structure.

Lattice constants

		a	b	c
1928 1962	Büssem and Herrmann [1]. National Bureau	$egin{array}{c} A \\ 7.52 \\ 7.510 \end{array}$	9. 44 9. 304	A 5. 89 5. 845 at
	of Standards.			25 °C

The lattice constants of Büssem and Herrmann were converted from kX to angstrom units for comparison with the NBS values.

The density of thallium perchlorate calculated from the NBS lattice constants is 4.940 g/cm<sup>3</sup> at

25 °C.

#### References

[1] W. Büssem and K. Herrmann, Röntgenographische Untersuchung der einwertigen Perchlorate, Z.
Krist. 67, 405–408 (1928).

[2] K. Herrmann and W. Ilge, Röntgenographische
Strukturerforschung der kubischen Modifikation der

Perchlorate, Z. Krist. 75, 41-66 (1930).
[3] H. Braekken and L. Harang, Die kubische Hochtemperaturstruktur einiger Perchlorate, Z. Krist. **75**, 538–549 (1930).

hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A				
	d	I			
110 020 101 111 120	A 5. 84 4. 65 4. 61 4. 14 3. 96	$\begin{array}{c} 4\\ 30\\ 54\\ 39\\ 19 \end{array}$			
200 021 210 121 211	3. 76 3. 64 3. 485 3. 278 2. 992	40 100 59 75 36			
$\begin{array}{c} 002,220 \\ 130 \\ 112,221 \\ 022 \\ 310 \\ \end{array}$	2. 922 2. 867 2. 614 2. 475 2. 417	$egin{array}{c} 40 \\ 11 \\ 21 \\ 9 \\ 6 \end{array}$			
230 122 040 202 311	2. 391 2. 350 2. 326 2. 306 2. 234	$\begin{array}{c} 3 \\ 24 \\ 4 \\ 6 \\ 78 \end{array}$			
140 231 041 222 132	2. 222 2. 213 2. 161 2. 066 2. 047	47 42 13 5 5			
330 103 400 113, 331 410	1. 9485 1. 8860 1. 8783 1. 8479 1. 8409	14 5 3 8 6			
023 142 411 123 213	1. 7970 1. 7688 1. 7552 1. 7480 1. 7001	$\begin{array}{c} 6 \\ 14 \\ 5 \\ 5 \\ 4 \end{array}$			
421 223, 332 251 402 412	1. 6681 1. 6212 1. 6036 1. 5793 1. 5572	$\begin{array}{c} 1 \\ 14 \\ 3 \\ < 1 \\ 8 \end{array}$			
060 431 303 313 233	1. 5501 1. 5485 1. 5374 1. 5167 1. 5107	10 12 4 8 6			
061 043, 350 510 161 004, 440	1. 4981 1. 4938 1. 4826 1. 4696 1. 4613	$   \begin{array}{c}     9 \\     9 \\     1 \\     9 \\     6   \end{array} $			
501	1. 4545	4			

## Yttrium Arsenate, YAsO<sub>4</sub> (tetragonal)

#### Powder Data cards

Card number	Index	Radiation	Source
2-0440	3. 39 1. 79 2. 60	Chromium	Strada and Schwendi- mann [1] 1934.

Additional published patterns. None.

NBS samples. The sample of yttrium arsenate was prepared at NBS by mixing solutions of yttrium chloride and sodium hydrogen arsenate. The precipitate was filtered, washed, and then heated to 750 °C. The yttrium chloride was obtained from the Lindsay Chemical Company, West Chicago, Ill. Their spectrographic analysis showed the presence of the following impurities in the chloride: a combined maximum as oxides of 0.1 percent of dysprosium and gadolinium and traces of terbium. Spectrographic analysis at NBS showed the following additional impurities in the arsenate: 0.1 to 1.0 percent of silicon; 0.01 to 0.1 percent of calcium and sodium; and 0.001 to 0.01 percent aluminum, boron, copper, iron, lead and magnesium.

The sample was colorless. The indices of refraction could not be determined because of the

small particle size.

The d-values of the three strongest lines are:

3.52, 2.661, and 1.8171 A.

Structural data. Strada and Schwendimann [1] in 1934 determined that yttrium arsenate has the zircon structure, the space group D<sub>4h</sub><sup>19</sup>—I4<sub>1</sub>/amd (No. 141) and 4 (YAsO<sub>4</sub>) per unit cell.

Lattice constants

		a	c
1934 1957 1962	Strada and Schwendimann [1]. Durif and Forrat [2] National Bureau of Standards.	A 6. 914 7. 06 7. 039	A 6. 293 6. 30 6. 292 at 25 °C

The density of yttrium arsenate calculated from the NBS lattice constants is 4.853 g/cm<sup>3</sup> at 25 °C.

-						
	hkl	1962 National Bureau of Standards Cu, 1.5405 A at 25 °C Internal standard, tungsten, a=3.1648 A				
		d .	I			
	200 112 220 202 301	A 3. 52 2. 661 2. 490 2. 347 2. 199 2. 010	100 73 18 5 6			
	321 312	1, 866 1, 817	$rac{4}{65}$			
	400	1. 760	16			
	420	1. 574	14			
	332 204 501 224 512	1. 468 1. 4359 1. 3737 1. 3293 1. 2644	$ \begin{array}{c} 16 \\ 11 \\ < 1 \\ 14 \\ 14 \end{array} $			
	440	1. 2446	4			
	$404,600 \\ 532$	1. 1731 1. 1272	$\begin{array}{c} 11 \\ 15 \end{array}$			
i	424, 620	1. 1128	15			
	116	1. 0258	6			
	$444,640 \\ 316,712 \\ 604 \\ 624 \\ 732$	0. 9760 . 9488 . 9404 . 9085 . 8867	$7 \\ 14 \\ 5 \\ 8 \\ 10$			
	800 820 516 644, 660	. 8799 . 8538 . 8349 . 8295	$\begin{array}{c} 3 \\ 3 \\ 10 \\ 7 \end{array}$			

#### References

[1] M. Strada and G. Schwendimann, La structura cristallina di alcuni fosfati dei metalli trivalenti. II. Arseniato e fosfato di ittrio, Gazz. chim. ital **64**, 662-674 (1934).

[2] A. Durif and F. Forrat, Sur quelques arséniates des terres rares à structure zircon, Compte rend. 245,

1636-1638 (1957).

## Zinc Tungstate, ZnWO<sub>4</sub> (monoclinic)

Powder Data cards. None.

Additional published patterns. None.

NBS sample. The sample of zinc tungstate was prepared at NBS by the reaction of solutions of zinc chloride and sodium tungstate. The precipitate was washed, dried, and heated to 1,000 °C for 10 min. Spectrographic analysis showed the following impurities: 0.01 to 0.1 percent of sodium and 0.001 to 0.01 percent of silicon.

The color of the sample was gray. The indices of refraction were not determined because the

sample was too fine-grained.

The d-values of the three strongest lines are:

2.931, 2.908, and 3.73 A.

Structural data. Broch [1] in 1929 determined that zinc tungstate has the magnesium tungstate structure, the space group  $C_{2h}^4$ —P2/c (No. 13), and  $2(ZnWO_4)$  per unit cell. The lattice constants of Broch have been converted from kX to angstrom units.

The density of zinc tungstate calculated from the NBS lattice constants is 7.870 g/cm<sup>3</sup> at 25 °C.

#### Reference

[1] E. K. Broch, Untersuchungen über Kristallstrukturen des Wolframittypus und des Scheelittypus, Skrifter Norsk. Videns.-Akad. Oslo I. Mat.-Naturv. Kl. No. 8 (1929).

hkl	1962 Nation of Stan Cu, 1.5405 A Internal st tungsten, a=	dards A at 25 °C andard,	
	d	I	
010 100 011 110 111	A 5. 72 4. 69 3. 73 3. 62 2. 931	10 35 38 37 100	
T11 020 021 002 120	2. 908 2. 859 2. 472 2. 464 2. 442	90 23 37 34 7	
$ \begin{array}{c} 200 \\ 121 \\ \underline{102} \\ 121 \\ 112 \end{array} $	2. 346 2. 192 2. 191 2. 183 2. 046	16 16 16 18 7	
$ \begin{array}{r}     \overline{1}12 \\     \underline{2}11 \\     \overline{2}11 \\     030 \\     022 \end{array} $	2. 029 1. 994 1. 978 1. 906 1. 866	$7 \\ 5 \\ 5 \\ 2 \\ 14$	
$ \begin{array}{r} 220 \\ 130 \\ \underline{122} \\ \overline{122} \\ 202, 221 \end{array} $	1. 813 1. 766 1. 740 1. 7290 1. 7074	$ \begin{array}{c} 13 \\ 21 \\ < 1 \\ < 1 \\ 26 \end{array} $	
$     \begin{array}{r}             \overline{2}21 \\             \overline{2}02 \\             \overline{1}31 \\             \overline{1}31 \\             212     \end{array} $	1. 6969 1. 6891 1. 6650 1. 6609 1. 6366	20 16 3 3 1	
013 300 032 113 113	1. 5778 1. 5634 1. 5076 1. 5007 1. 4903	5 1 6 12 11	
$ \begin{array}{r} 230 \\ \underline{222} \\ \overline{2}22 \\ 311 \\ \overline{3}11, 132 \end{array} $	1. 4792 1. 4662 1. 4541 1. 4465 1. 4379	3 5 6 10 19	
$     \begin{array}{r}             \hline             132 \\             023 \\             041 \\             123 \\             \hline             123     \end{array} $	1. 4326 1. 4236 1. 3732 1. 3663 1. 3589	17 11 10 <1 1	

#### Lattice constants

		a	b	c	β
1930 1962	Broch [1] National Bureau of Standards	A 4. 69 4. 691	A 5. 74 5. 720	A 4. 96 4. 925	89. 50° 89. 36 at 25 °C

# CUMULATIVE INDEX TO CIRCULAR 539, VOLUMES 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, MONO-GRAPH 25, SECTION 1 AND SECTION 2 5

	Vol. or			Wal or	
	sec.	Page		Vol. or sec.	Page
Aluminum, Al	1	11	Arsenic, As	3	6
Aluminum antimony, AlSb	4	72	Arsenic (III) iodide, AsI <sub>3</sub>	6	17
Aluminum calcium sulfate hydrate (ettring-	0		Arsenic trioxide (arsenolite), As <sub>2</sub> O <sub>3</sub>	1	$\frac{51}{7}$
ite), Al <sub>2</sub> O <sub>3</sub> ·6CaO·3SO <sub>3</sub> ·31H <sub>2</sub> O	8	3	Barium, Ba	$^{ m 4}_{ m 2m}$	$\frac{7}{6}$
Aluminum chloride hexahydrate (chlor-	7	3	Barium carbonate (witherite), $BaCO_3$	$\frac{z_{\rm m}}{2}$	$\frac{6}{54}$
aluminite), AlCl <sub>3</sub> ·6H <sub>2</sub> OAluminum fluosilicate, topaz, Al <sub>2</sub> SiO <sub>4</sub> (F,	•	9	Barium carbonate, BaCO <sub>3</sub> (cubic)	10	11
OH),	1m	4	Barium fluoride, BaF <sub>2</sub>	1	70
$OH)_2$ Aluminum metaphosphate, $Al(PO_3)_3$	2m	3	Barium molybdate, BaMoO <sub>4</sub>	7	7
Aluminum orthophosphate (berlinite),			Barium nitrate (nitrobarite), Ba(NO <sub>3</sub> ) <sub>2</sub>	1	81
AlPO <sub>4</sub> (trigonal)Aluminum orthophosphate, AlPO <sub>4</sub> (ortho-	10	3	Barium perchlorate trihydrate, Ba(ClO <sub>4</sub> ) <sub>2</sub> .	0	_
Aluminum orthophosphate, AlPO <sub>4</sub> (ortho-	10	4	3H <sub>2</sub> O	$2 \mathrm{m}$	7
rhombic)Aluminum oxide, alpha (corundum), Al <sub>2</sub> O <sub>3</sub>	$\frac{10}{9}$	$\frac{4}{3}$	Barium peroxide, BaO <sub>2</sub> Barium sulfate (barite), BaSO <sub>4</sub>	$\frac{6}{3}$	$\begin{array}{c} 18 \\ 65 \end{array}$
Aluminum oxide monohydrate, alpha (böh-	θ	9	Barium sulfide, BaS	7	8
mite) Al <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> O	3	38	Barium titanate, BaTiO <sub>3</sub>	$\frac{7}{3}$	45
mite) Al <sub>2</sub> O <sub>3</sub> ·H <sub>2</sub> OAluminum oxide monohydrate, beta (dia-			Barium tungstate, BaWO <sub>4</sub>	7	9
spore), $Al_2O_3 \cdot H_2O_{}$	3	41	Barium zirconate, BaZrO <sub>3</sub>	5	8
Ammonium aluminum sulfate dodecahy-	0	0	Beryllium aluminum oxide (chrysoberyl),		
drate, NH <sub>4</sub> Al(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	$\frac{6}{9}$	3	BeAl <sub>2</sub> O <sub>4</sub> Beryllium aluminum silicate (beryl) Be <sub>3</sub> Al <sub>2</sub>	9	10
Ammonium azide, NH <sub>4</sub> N <sub>3</sub>	9	4	Berymum aruminum sincate (beryi) $Be_3AI_2$	9	13
(NH <sub>4</sub> )HCO <sub>3</sub>	9	5	$(\dot{\mathrm{Si}}\mathrm{O_3})_{6}$ Beryllium chromium oxide, Be $\mathrm{Cr_2O_4}$	10	$\frac{13}{12}$
Ammonium bomide, NH <sub>4</sub> Br	$\overset{\circ}{2}$	49	Beryllium germanate, Be <sub>2</sub> GeO <sub>4</sub>	10	13
Ammonium bromoosmate, (NH <sub>4</sub> )OsBr <sub>6</sub>	$\frac{2}{3}$	71	Beryllium orthosilicate (phenacite), Be <sub>2</sub> SiO <sub>4</sub>	8	11
Ammonium bromoplatinate, (NH <sub>4</sub> ) <sub>2</sub> PtBr <sub>6</sub>	9	6	Beryllium oxide (bromellite), BeO	1	36
Ammonium bromoselenate, (NH <sub>4</sub> ) <sub>2</sub> SeBr <sub>6</sub>	8	4	Bismuth, Bi Bismuth fluoride, BiF <sub>3</sub>	3	20
Ammonium bromotellurate, (NH <sub>4</sub> ) <sub>2</sub> TeBr <sub>6</sub>	8	5	Bismuth fluoride, BiF <sub>3</sub>	1m	7
Ammonium chloride (sal-ammoniac),	-1	50	Bismuth (III) iodide, BiI <sub>3</sub>	6	20
NH <sub>4</sub> ClAmmonium chloroiridate (NH <sub>4</sub> ) <sub>2</sub> IrCl <sub>6</sub>	$\frac{1}{8}$	$\begin{array}{c} 59 \\ 6 \end{array}$	Bismuth oxybromide, BiOBrBismuth oxychloride (bismoclite), BiOCl	8 4	$\begin{array}{c} 14 \\ 54 \end{array}$
Ammonium chloroosmate, (NH <sub>4</sub> ) <sub>2</sub> OsCl <sub>6</sub>	$1 \mathrm{m}$	6	Bismuth oxygodide, BiOI	9	$\frac{34}{16}$
Ammonium chloropalladate, (NH <sub>4</sub> ) <sub>2</sub> PdCl <sub>6</sub>	8	7.	Bismuth sulfide (bismuthinite), Bi <sub>2</sub> S <sub>3</sub>	4	23
Ammonium chloropalladite, (NH <sub>4</sub> ) <sub>2</sub> PdCl <sub>4</sub>	6	6	Cadmium, Cd	3	10
Ammonium chloroplatinate, (NH <sub>4</sub> ) <sub>2</sub> PtCl <sub>6</sub>	5 5	3	Cadmium bromide, CdBr <sub>2</sub>	9	17
Ammonium chlorostannate (NH <sub>4</sub> ) <sub>2</sub> SnCl <sub>6</sub>	5	4	Cadmium carbonate (otavite), CdCO <sub>3</sub>	7	11
Ammonium chlortellurate, (NH <sub>4</sub> ) <sub>2</sub> TeCl <sub>6</sub>	8	8	Cadmium chloride, CdCl <sub>2</sub>	9	18
Ammonium chromium sulfate dodecahy-	c	7	Cadmium cyanide, Cd(CN) <sub>2</sub> Cadmium molybdate, CdMoO <sub>4</sub>	$2 \mathrm{m}$	8
drate, NH <sub>4</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> OAmmonium dihydrogen phosphate,	6	7	Cadmium oxide, CdO	$rac{6}{2}$	$\begin{array}{c} 21 \\ 27 \end{array}$
NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	4	64	Cadmium selenide, CdSe, (hexagonal)	$\tilde{7}$	12
Ammonium fluogermanate, (NH <sub>4</sub> ) <sub>2</sub> GeF <sub>6</sub>	$\hat{6}$	8	Cadmium sulfide (greenockite), CdS	$\dot{4}$	$1\overline{5}$
Ammonium fluosilicate (cryptohalite),			Cadmium tungstate, CdWO <sub>4</sub>	2m	8
(NH <sub>4</sub> ) <sub>2</sub> SiF <sub>6</sub> Ammonium gallium sulfate dodecahydrate,	5	5	tri-Calcium aluminate, 3CaO·Al <sub>2</sub> O <sub>3</sub>	5	10
Ammonium gallium sulfate dodecahydrate,	0	0	Calcium aluminate 12:7, 12CaO·7Al <sub>2</sub> O <sub>3</sub>	9	20
NH <sub>4</sub> Ga(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	6	9	Calcium aluminum germanate, Ca <sub>3</sub> Al <sub>2</sub>	10	15
Ammonium iodide, NH, I	4	56	(GeO <sub>4</sub> ) <sub>3</sub> Calcium bromide hexahydrate, CaBr <sub>2</sub> ·6H <sub>2</sub> O_	$\frac{10}{8}$	$\frac{15}{15}$
NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	6	10	Calcium carbonate (aragonite), CaCO <sub>3</sub>	$\frac{3}{3}$	53
NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O <sub></sub> Ammonium metavanadate, NH <sub>4</sub> VO <sub>3</sub>	8	9	Calcium carbonate (calcite) CaCO <sub>3</sub>	$\frac{3}{2}$	51
Ammonium nitrate (ammonia-niter),			Calcium chromate, CaCrO <sub>4</sub>	7	13
NH <sub>4</sub> NO <sub>3</sub>	7	4	Calcium chromium germanate. Ca <sub>3</sub> Cr <sub>2</sub>		
Ammonium oxalate monohydrate (oxam-	_		(GeO <sub>4</sub> ) <sub>3</sub> Calcium chromium silicate (uvarovite),	10	16
mite), (NH <sub>4</sub> ) <sub>2</sub> C <sub>2</sub> O <sub>4</sub> ·H <sub>2</sub> O	7	5	Calcium chromium silicate (uvarovite),	10	17
Ammonium perchlorate, NH <sub>4</sub> ClO <sub>4</sub> , (orthorhombic)	7	6	$ m Ca_3Cr_2(SiO_4)_3$ ————————————————————————————————————	$10 \\ 1$	$\frac{17}{69}$
Ammonium perrhenate, NH <sub>4</sub> ReO <sub>4</sub>	9	7	Calcium formate, $Ca(HCO_2)_2$	8	16
Ammonium phosphomolybdate tetrahy-	U	•	Calcium gallium germanate, Ca <sub>3</sub> Ga <sub>2</sub> (GeO <sub>4</sub> ) <sub>3-</sub>	$1\overset{\circ}{0}$	18
drate, $(NH_4)_3 PO_4 (M_0O_3)_{12} \cdot 4H_2O_{}$	8	10	Calcium hydroxide (portlandite), Ca(OH) <sub>2</sub>	1	58
Ammonium sulfate (mascagnite), (NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>			Calcium iron germanate, $Ca_3Fe_2(GeO_4)_{3}$	10	19
(revised)	9	8	Calcium iron silicate (andradite),		2.2
Ammonium zirconium fluoride (NH <sub>4</sub> ) <sub>3</sub> ZrF <sub>7</sub>	6	14	$\mathrm{Ca_3Fe_2Si_3O_{12}}$	9	22
Antimony, Sb	$^{ m 3}_{ m 2m}$	$\frac{14}{4}$	Calcium molybdate (powellite), CaMoO <sub>4</sub> Calcium nitrate, Ca(NO <sub>3</sub> ) <sub>2</sub>	$\frac{6}{7}$	$\begin{array}{c} 22 \\ 14 \end{array}$
Antimony (III) iodide, SbI <sub>3</sub>	6	16	Calcium oxide, CaO	í	43
Antimony (III) oxide (senarmontite), Sb <sub>2</sub> O <sub>3</sub>	3	31	Calcium sulfate (anhydrite), CaSO <sub>4</sub>	4	65
Antimony (III) oxide, valentinite, Sb <sub>2</sub> O <sub>3</sub>	10	$\overset{\circ}{6}$	Calcium sulfide (oldhamite), CaS	7	15
Antimony (IV) oxide (cervantite), Sb <sub>2</sub> O <sub>4</sub>	10	8	Calcium tungstate (scheelite), CaWO <sub>4</sub>	6	23
Antimony (V) oxide, Sb <sub>2</sub> O <sub>5</sub>	10	10	Carbon (diamond), C	2	5
Antimony (III) sulfide (stibnite), Sb <sub>2</sub> S <sub>3</sub>	5	6	Cerium (III) chloride, CeCl <sub>3</sub>	$1 \mathrm{m}$	8
<sup>5</sup> Further work on this program is in progress, and it is a additional sections will be issued. Therefore, the accumulation is not necessarily the concluding index for the project.	anticipate	d that	Cerium (III) fluoride, CeF <sub>3</sub> Cerium magnesium nitrate 24-hydrate,	8	17
is not necessarily the concluding index for the project.	avaro mut	A ACTO	Cerium magnesium intrate 24-nydrate, $Ce_2Mg_3(NO_3)_{12}\cdot 24H_2O_{}$	10	20
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	Vol. or	<b>T</b>		Vol. or	
Cerium(IV) oxide (ceriamite) CeO <sub>2</sub>	sec.	Page 56	Gallium antimonide, GaSb	sec.	Page 30
Cerium(III) vanadate, CeVO <sub>4</sub>	1m	9	Gallium oxide, alpha, $Ga_2O_3$	4	25
Cesium aluminum sulfate dodecahydrate,		۰. ۳	Gallium phosphate, (α-quartz type) GaPO <sub>4</sub>	8	27
$ ext{CsAl}(SO_4)_2 \cdot 12H_2O$ Cesium bromate, $CsBrO_3$	6	$\begin{array}{c} 25 \\ 18 \end{array}$	Germanium, Ge Germanium dioxide, GeO <sub>2</sub> (hexagonal)	1	18 51
Cesium bomide, CsBr	3	49	Germanium dioxide, GeO <sub>2</sub> (hexagonal)	8	28
Cesium bomide, CsBr Cesium bromoosmate(IV), Cs <sub>2</sub> OsBr <sub>6</sub>	2m	10	Germanium(IV) iodide, GeI <sub>4</sub>	$\ddot{5}$	25
Cesium bromoplatinate, Cs <sub>2</sub> PtBr <sub>6</sub>	8	19	Gold, Au	$\frac{1}{7}$	33
Cesium bromoselenate, Cs <sub>2</sub> SeBr <sub>6</sub> Cesium bromotellurate, Cs <sub>2</sub> TeBr <sub>6</sub>	8 9	$\frac{20}{24}$	Gold antimony 1:2 (aurostibite), AuSb <sub>2</sub> Gold(I) cyanide, AuCN	10	18 33
Cesium chlorate, CsClO <sub>3</sub>	8	$\tilde{20}$	Gold tin 1:1 AuSn	7	19
Cesium chloride, CsCl	2	44	Hafnium, Hf	3	18
Cesium chloroosmate (IV), Cs <sub>2</sub> OsCl <sub>6</sub> Cesium chloroplatinate, Cs <sub>2</sub> PtCl <sub>6</sub>	$\frac{2\mathrm{m}}{5}$	11 14	$\begin{array}{ccc} Holmium & ethylsulfate & nonahydrate, \\ Ho[(C_2H_5)SO_4]_3 \cdot 9H_2O_{} \end{array}$	1	10
Cesium chlorostannate, Cs <sub>2</sub> FtCl <sub>6</sub>	5	$\frac{14}{16}$	Holmium sesquioxide, $Ho_2O_3$	1m 9	$\begin{array}{c} 18 \\ 32 \end{array}$
Cesium chromium sulfate dodecahydrate,	Ť	10	Indium, In	$\ddot{3}$	12
$C_{\rm s}C_{\rm r}({ m SO_4})_2\cdot 12{ m H_2O}$	8	21	Indium antimony, InSb	4	73
Cesium dichloroiodide, CsICl <sub>2</sub>	3 8	$\begin{array}{c} 50 \\ 22 \end{array}$	Indium oxide, $In_2O_3$ Indium phosphate, $InPO_4$	5	$\frac{26}{29}$
Cesium fluogermanate, Cs <sub>2</sub> GeF <sub>6</sub>	5	$\frac{22}{17}$	Iodic acid, HIO <sub>3</sub>	5	28
Cesium fluoplatinate, Cs <sub>2</sub> PtF <sub>6</sub>	6	27	lodine, $I_2$	3	16
Cesium fluosilicate, Cs <sub>2</sub> SiF <sub>6</sub>	5	19	Iridium, Ir	4	9
Cesium gallium sulfate dodecahydrate, CsGa(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	8	23	Iron, Alpha, FeIron arsenide, FeAs	4 1m	$\begin{array}{c} 3 \\ 19 \end{array}$
Cesium iodide, CsI	4	$\frac{23}{47}$	Iron arsenide (loellingite), FeAs <sub>2</sub>	10	34
Cesium iron sulfate dodecahydrate,			Iron sulfide (pyrite). FeS <sub>2</sub>	5	29
$CsFe(SO_4)_2 \cdot 12H_2O$	6	28	Lanthanum borate, LaBO <sub>3</sub>	$1^{\mathrm{m}}$	20
Cesium nitrate, CsNO <sub>3</sub>	$^{9}_{1 m m}$	$\begin{array}{c} 25 \\ 10 \end{array}$	Lanthanum chloride, $LaCl_3$	$\frac{1}{7}$	$\frac{21}{21}$
Cesium sulfate, Cs <sub>2</sub> SO <sub>4</sub>	7	17	Lanthanum magnesium nitrate 24-hydrate,	•	21
Cesium vanadium sulfate dodecahydrate,			$La_2Mg_3(NO_3)_{12} \cdot 24H_2O_{}$	$1 \mathrm{m}$	22
$\mathrm{CsV}(\mathrm{SO_4})_2\cdot 12\mathrm{H_2O}$	1m	11	Lanthanum oxide, La <sub>2</sub> O <sub>3</sub> Lanthanum oxychloride, LaOCl	$\frac{3}{2}$	33
Chromium, CrChromium orthophosphate, alpha, CrPO <sub>4</sub>	$^{5}_{2 m m}$	$\frac{20}{12}$	Lead, Pb	$\frac{7}{1}$	$\begin{array}{c} 22 \\ 34 \end{array}$
Chromium orthophosphate, beta, CrPO <sub>4</sub>	9	$\frac{12}{26}$	Lead bromide, PbBr <sub>2</sub>	2	47
Chromium(III) oxide, $Cr_2O_3$	5	22	Lead carbonate (cerrussite), PbCO <sub>3</sub>	$^2$	56
Chromium silicide, Cr <sub>3</sub> Si	6	29	Lead chloride (cotunnite), PbCl <sub>2</sub>	2	45
Cobalt aluminum oxide, CoAl <sub>2</sub> O <sub>4</sub> Cobalt arsenide (skutterudite), CoAs <sub>3</sub>	$\frac{9}{10}$	$\begin{array}{c} 27 \\ 21 \end{array}$	Lead formate, Pb(HCO <sub>2</sub> ) <sub>2</sub> Lead fluochloride (matlockite) PbFCl	8	$\begin{array}{c} 30 \\ 76 \end{array}$
Cobalt(II) carbonate (spherocobaltite),	10	21	Lead fluoride, alpha, PbF <sub>2</sub>	5	31
$C_0CO_3$	10	24	Lead fluoride, beta, PbF <sub>2</sub>	5	33
Cobalt diarsenide, CoAs <sub>2</sub>	10	26	Lead(II), iodide, PbI <sub>2</sub>	$\frac{5}{5}$	34
Cobalt gallate, $CoGa_2O_4$ ————————————————————————————————————	$\frac{10}{10}$	$\begin{array}{c} 27 \\ 27 \end{array}$	Lead molybdate (wulfenite), PbMoO <sub>4</sub> Lead monoxide (litharge), PbO (red)	2	$\begin{array}{c} 23 \\ 30 \end{array}$
Cobalt iron arsenide (safflorite), CoFeAs <sub>4</sub>	10	$\frac{27}{28}$	Lead monoxide (massicot) PbO (yellow)	$\tilde{2}$	32
Cobalt mercury thiocyanate, Co[Hg(CNS) <sub>4</sub> ]_	2m	13	Lead nitrate, Pb(NO <sub>3</sub> ) <sub>2</sub> Lead(II, III) oxide (minimum), Pb <sub>3</sub> O <sub>4</sub>	5	36
Cobalt(II) oxide, CoO	9	28		8	32
Cobalt (II, III) oxide, $Co_3O_4$	$^{9}_{2 m m}$	$\frac{29}{14}$	Lead phosphate hydrate (lead hydroxyapa- tite), Pb <sub>5</sub> (PO <sub>4</sub> ) <sub>3</sub> OH	8	33
Copper, Cu	1	10	Lead selenide (clausthalite), PbSe	5	38
Copper, CuCopper(I) bromide, CuBr	4	36	Lead sulfate (anglesite), PbSO <sub>4</sub>	3	67
Copper carbonate, basic, (azurite), Cu <sub>3</sub> (OH) <sub>2</sub>	10	20	Lead sulfide (galena), PbS	$\frac{2}{5}$	18 39
$(CO_3)_2$ Copper carbonate, basic, (malachite),	10	30	Lead titanate, PbTiO <sub>3</sub> Lead tungstate (stolzite), PbWO <sub>4</sub>	7	$\frac{39}{24}$
$\mathrm{Cu}_2(\mathrm{OH})_2(\mathrm{CO}_3)_{}$	10	31	Lithium arsenate, Li <sub>3</sub> AsO <sub>4</sub>	$2\mathrm{m}$	19
Copper(I) chloride (nantokite), CuCl	4	35	Lithium bromide, LiBr	4	30
Copper(I) iodide (marshite), CuI	$rac{4}{2}$	$\frac{38}{23}$	Lithium chloride, LiClLithium fluoride, LiF	1 1	$\frac{62}{61}$
Copper(I) oxide (cuprite), Cu <sub>2</sub> O Copper(II) oxide (tenorite), CuO	1	$\frac{23}{49}$	Lithium iodate, LiIO <sub>3</sub>	$\frac{1}{7}$	26
Copper(II) sulfide (covellite), CuS	$\overline{4}$	13	Lithium molybdate, Li <sub>2</sub> MoO <sub>4</sub> , (trigonal)	1m	23
Dysprosium gallium oxide 3:5, Dy <sub>3</sub> Ga <sub>2</sub>	0		Lithium oxide, Li <sub>2</sub> O	1m	25
$(GaO_4)_3$	$\frac{2\mathrm{m}}{9}$	$\begin{array}{c} 15 \\ 30 \end{array}$	Lithium nitrate, LiNO <sub>3</sub> Lithium perchlorate trihydrate, LiClO <sub>4</sub> ·3H <sub>2</sub> O	7 8	$\begin{array}{c} 27 \\ 34 \end{array}$
Erbium gallium oxide 3:5, $\text{Er}_3\text{Ga}_2(\text{GaO}_4)_{3}$	$1 \mathrm{m}^{9}$	12	Lithium trimetaphosphate trihydrate,	0	01
Erbium manganite, ErMnO <sub>3</sub>	2m	16	Li <sub>3</sub> P <sub>3</sub> O <sub>9</sub> ·3H <sub>2</sub> O Lithium tungstate, Li <sub>2</sub> WO <sub>4</sub> , (trigonal)	2m	20
Erbium phosphate, ErPO <sub>4</sub>	9	31	Lithium tungstate, Li <sub>2</sub> WO <sub>4</sub> , (trigonal)	$1 \mathrm{m}$	25
Erbium sesquioxide, Er <sub>2</sub> O <sub>3</sub> Europium(III) chloride, EuCl <sub>3</sub>	$\frac{8}{1 \mathrm{m}}$	$\begin{array}{c} 25 \\ 13 \end{array}$	Lithium tungstate hemihydrate, Li <sub>2</sub> WO <sub>4</sub> .	2m	20
Europium gallium oxide 3:5, Eu <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>	$2^{\mathrm{m}}$	$\frac{13}{17}$	Lutetium gallium oxide $3:5$ , Lu <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>	$2^{\mathrm{m}}$	22
Europium oxychloride, EuOCl	1m	13	Lutetium manganite, LuMnO <sub>3</sub>	2m	23
Gadolinium fluoride, GdF <sub>3</sub>	$1 \mathrm{m}$	14	Lutetium oxide, Lu <sub>2</sub> O <sub>3</sub>	1m	27
Gadolinium gallium oxide 3:5, Gd <sub>3</sub> Ga <sub>2</sub>	$2 \mathrm{m}$	18	Magnesium, Mg Magnesium aluminate (spinel), MgAl <sub>2</sub> O <sub>4</sub>	$\frac{1}{2}$	10 35
$(GaO_4)_3$ Gadolinium oxide, $Gd_2O_3$	$1 \mathrm{m}$	16	Magnesium aluminum silicate (low-cordi-		00
Gadolinium oxychloride, GdOCl	1m	17	erite), $Mg_2Al_4Si_5O_{18}$ (orthorhombic)	$1 \mathrm{m}$	28
Gallium, Ga	2	9	Magnesium aluminum silicate (high-cordi-	1 m	29
m_Monograph 95			erite), Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub> (hexagonal) Magnesium carbonate (magnesite), MgCO <sub>3</sub> _	$\frac{1}{7}$	$\frac{29}{28}$
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	Vol. or			Vol. or	
Magnesium abromita (nianashramita)	sec.	Page	Distinum Dt	sec.	Page 31
Magnesium chromite (picrochromite),	9	34	Platinum, PtPotassium aluminum sulfate dodecahydrate,	1	31
MgCr <sub>2</sub> O <sub>4</sub> Magnesium fluoride (sellaite), MgF <sub>2</sub>	4	33	$KAl(SO_4)_2 \cdot 12H_2O_{}$	6	36
Magnesium gallate, MgGa <sub>2</sub> O <sub>4</sub>	10	36	Potassium borohydride, KBH <sub>4</sub>	$\tilde{9}$	44
Magnesium germanate, Mg <sub>2</sub> GeO <sub>4</sub> (cubic)	$\overline{10}$	37	Potassium bromate, KBrO <sub>3</sub>	7	38
Magnesium germanate, Mg <sub>2</sub> GeO <sub>4</sub> (ortho-			Potassium bromide, KBr	1	66
rhombic)	10	38	Potassium bromoplatinate, K. PtBr6	8	40
Magnesium hydroxide (brucite), Mg(OH) <sub>2</sub>	6	30	Potassium bromoselenate, K <sub>2</sub> SeBr <sub>6</sub>	8	41
Magnesium oxide (periclase), MgO Magnesium silicate (enstatite), MgSiO <sub>3</sub>	$\frac{1}{6}$	$\begin{array}{c} 37 \\ 32 \end{array}$	Potassium chloride (sylvite), KCl Potassium chloroplatinate, K <sub>2</sub> PtCl <sub>6</sub>	$\frac{1}{5}$	$\frac{65}{49}$
Magnesium silicate (enstatite), Mg <sub>2</sub> SiO <sub>4</sub>	1	83	Potassium chlororhenate, $K_2$ ReCl <sub>6</sub>	$2\mathrm{m}$	28
Magnesium silicate fluoride (norbergite)	-	00	Potassium chlororuthenate (IV), K <sub>2</sub> RuCl <sub>6</sub>	10	46
Mg <sub>2</sub> SiO <sub>4</sub> ·MgF <sub>2</sub>	10	39	Potassium chlorostannate K <sub>2</sub> SnCl <sub>6</sub>	6	38
Magnesium silicate fluoride (humite).			Potassium chromium sulfate dodecahydrate,		
$3 \mathrm{Mg}_2 \mathrm{SiO}_4 \cdot \mathrm{MgF}_2$	$1 \mathrm{m}$	30	$KCr(SO_4)_2 \cdot 12H_2O_{}$ Potassium cobaltinitrite, $K_3Co(NO_2)_{6}$	6	39
Magnesium sulfate heptahydrate (epsomite),	77	20	Potassium cobaltinitrite, K <sub>3</sub> Co(NO <sub>2</sub> ) <sub>6</sub>	$\frac{9}{7}$	$\frac{45}{39}$
MgSO <sub>4</sub> ·H <sub>2</sub> O	7 7	$\frac{30}{31}$	Potassium cyanate, KCNOPotassium cyanide, KCN	1	39 77
Magnesium tin, Mg <sub>2</sub> Sn	5	41	Potassium dihydrogen arsenate, KH <sub>2</sub> AsO <sub>4</sub>	$1 \mathrm{m}$	38
Magnesium titanate (geikielite), MgTiO <sub>3</sub>	5	43	Potassium dihydrogen phosphate, KH <sub>2</sub> PO <sub>4</sub>	3	69
Magnesium tungstate, MgWO <sub>4</sub>	1	84	Potassium fluogermanate, K <sub>2</sub> GeF <sub>6</sub>	6	41
Manganese aluminate (galaxite), MnAl <sub>2</sub> O <sub>4</sub>	9	35	Potassium fluoplatinate, K <sub>2</sub> PtF <sub>6</sub>	6	42
Manganese(II) carbonate (rhodochrosite),	) <del></del> 7	9.0	Potassium fluoride, KF	1	64
MnCO <sub>3</sub>	7 9	$\begin{array}{c} 32 \\ 36 \end{array}$	Potassium fluosilicate (hieratite), K <sub>2</sub> SiF <sub>6</sub>	5	$\frac{50}{40}$
Manganese ferrite (jacobsite), MnFe <sub>2</sub> O <sub>4</sub> Manganese(II) oxide (manganosite), MnO	5	45	Potassium fluotitanate, K <sub>2</sub> TiF <sub>6</sub> ————————————————————————————————————	á	46
Manganese (III) oxide (partridgeite), Mn <sub>2</sub> O <sub>3</sub>	9	37	Potassium hydroxy-chlororuthenate,	J	10
Manganese selenide, MnSe	10	41	$K_4Ru_2Cl_{10}O \cdot H_2O_{}$	10	47
Manganese sulfide, alpha (alabandite).			Potassium iodide, KI	1	68
MnS Manganese(II) tungstate (huebnerite),	4	11	Potassium metaperiodate, KIO <sub>4</sub>	7	41
Manganese (11) tungstate (huebnerite),	0	0.4	Potassium nitrate (niter), KNO <sub>3</sub>	3	58
$MnWO_4$ Mercury(I) bromide, $Hg_2Br_2$	$rac{2 ext{m}}{7}$	$\frac{24}{33}$	Potassium nitroso chlororuthenate, K <sub>2</sub> RuCl <sub>6</sub> -NO	2m	29
Mercury (I) chloride (calomel), Hg <sub>2</sub> Cl <sub>2</sub>	í	72	Potassium perchlorate, KClO <sub>4</sub>	$rac{2 ext{m}}{6}$	$\frac{23}{43}$
Mercury (II) chloride, HgCl <sub>2</sub>	i	73	Potassium permanganate, KMnO <sub>4</sub>	7	42
Mercury(II) cyanide, Hg(CN) <sub>2</sub>	$\bar{6}$	35	Potassium perrhenate, KReO <sub>4</sub>	8	41
Mercury (II) fluoride, HgF <sub>2</sub>	$2 \mathrm{m}$	25	Potassium phosphomolybdate, tetrahydrate,		
Mercury (I) iodide, HgI	4	49	$K_2PO_4(MoO_3)_{12}\cdot 4H_2O_{}$	8	43
Mercury (II) iodide, HgI <sub>2</sub> Mercury (II) oxide (montroydite), HgO	1	74	Potassium sulfate (arcanite), K <sub>2</sub> SO <sub>4</sub>	3 8	62 44
(revised)	9	39	Potassium thiocyanate, KCNS Potassium zinc fluoride, KZnF <sub>3</sub>	5	$\frac{44}{51}$
Mercury (II) selenide (tiemannite), HgSe	7	35	Praseodymium chloride, PrCl <sub>3</sub>	$1 \mathrm{m}$	39
Mercury(II) sulfide (cinnabar), HgS (hex-	•	33	Praseodymium fluoride, PrF <sub>3</sub>	5	52
agonal)	4	17	Praseodymium fluoride, PrF <sub>3</sub>	9	47
Mercury(II) sulfide (metacinnabar), HgS		0.1	Rhenium, Re	$\frac{1}{2}$	13
(cubic)	4	21	Rhodium, Rh	3	9
Molybdenum, MoMolybdenite), MoS <sub>2</sub> _	$\frac{1}{5}$	$\frac{20}{47}$	Rubidium aluminum sulfate dodecahydrate, RbAl(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O <sub></sub>	6	44
Molybdenum trioxide (molybdite), MoO <sub>3</sub>	3	30	Rubidium bromate, $RbBrO_3$	8	45
Neodymium borate, NdBO <sub>3</sub>	$1 \mathrm{m}$	$\frac{32}{32}$	Rubidium bromide, RbBr	$\ddot{7}$	43
Neodymium chloride, NdCl <sub>3</sub>	$1 \mathrm{m}$	33	Rubidium bromotellurate, Rb <sub>2</sub> TeBr <sub>6</sub>	8	46
Neodymium ethylsulfate nonahydrate,			Rubidium chlorate, RbClO <sub>3</sub>	8	47
$\operatorname{Nd}[(C_2H_5)SO_4]_3 \cdot 9H_2O$	9	41	Rubidium chloride, RbCl	$\frac{4}{2}$	41
Neodymium fluoride, NdF <sub>3</sub>	8	36	Rubidium chloroplatinate, Rb <sub>2</sub> PtCl <sub>6</sub> Rubidium chlorostannate, Rb <sub>2</sub> SnCl <sub>6</sub>	$\frac{5}{6}$	53 46
$(G_3O_4)_2$	$1 \mathrm{m}$	34	Rubidium chlorotellurate, $Rb_2SnCl_6$	8	48
$(GaO_4)_3$ Neodymium oxide, $Nd_2O_3$	4	26	Rubidium chromium sulfate dodecahydrate,	O	10
Neodymium oxychloride, NdOCl	8	37	$RbCr(SO_4)_2 \cdot 12H_2O_{}$	6	47
Nickel, Ni	1	13	Rubidium fluoplatinate, Rb <sub>2</sub> PtF <sub>6</sub>	6	48
Nickel aluminate, NiAl <sub>2</sub> O <sub>4</sub>	9	42	Rubidium fluosilicate, Rb <sub>2</sub> SiF <sub>6</sub>	6	49
Nickel arsenic 1: 2 (rammelsbergite) NiAs <sub>2</sub>	10	42	Rubidium iodide, RbI	22	$\frac{43}{30}$
Nickel arsenic sulfide (gersdorffite) NiAsS Nickel (II) carbonate, NiCO <sub>3</sub> (trigonal)	$1\mathrm{m} \ 1\mathrm{m}$	$\begin{array}{c} 35 \\ 36 \end{array}$	Rubidium perchlorate, RbClO <sub>4</sub> Rubidium periodate, RbIO <sub>4</sub>	$rac{2 ext{m}}{2 ext{m}}$	31
Nickel ferrite (trevorite), NiFe <sub>2</sub> O <sub>4</sub>	10	44	Rubidium sulfate, Rb <sub>2</sub> SO <sub>4</sub>	8	48
Nickel fluosilicate hexahydrate, NiSiF <sub>6</sub> ·6 <sub>2</sub> HO	8	38	Ruthenium, Ru	$\overline{4}$	5
Nickel gallate, NiGa <sub>2</sub> O <sub>4</sub>	10	45	Samarium chloride, SmCl <sub>3</sub>	$1 \mathrm{m}$	40
Nickel germanate, Ni <sub>2</sub> GeO <sub>4</sub>	9	43	Samarium fluoride, SmF <sub>3</sub>	$1 \mathrm{m}$	41
Nickel (II) oxide (bunsenite), NiO	1	47	Samarium gallium oxide 3:5, Sm <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub> .	$1 \mathrm{m}$	42
Nickel sulfate, NiSO <sub>4</sub>	$\frac{2\mathrm{m}}{7}$	$\frac{26}{36}$	Samarium oxychloride, SmÓCl	$\frac{1 ext{m}}{3}$	$\begin{array}{c} 43 \\ 27 \end{array}$
Nickel sulfide, millerite, NiS	$1 \mathrm{m}^{\prime}$	$\frac{30}{37}$	Scandium oxide, $Sc_2O_3$ Scandium phosphate, $ScPO_4$	8	50
Nickel Tungstate, NiWO <sub>4</sub>	$2^{\mathrm{m}}$	27	Selenium, Se	5	54
Niobium silicide, NbSi <sub>2</sub>	8	$\frac{1}{39}$	Selenium dioxide (selenolite), SeO <sub>2</sub>	1	53
Osmium, Os	4	8	Silicon, Si	$^2$	6
Palladium, Pd	1	21	Silicon dioxide (alpha or low quartz), SiO <sub>2</sub>	3	24
Palladium oxide, PdO	4	27	Silicon dioxide (alpha or low cristobalite),		
m—Monograph 25.			$SiO_2$ (Revised)	10	48

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Silicon dioxide (beta or high crisobalite),	sec.	rage	Tellurium(IV) oxide, paratellurite, TeO <sub>2</sub>	sec. 10	Page 55
$\mathrm{SiO}_2$	1	42	Tellurium (IV) oxide (tellurite), TeO <sub>2</sub> (ortho-	0	E17
Silver, AgSilver arsenate, Ag <sub>3</sub> AsO <sub>4</sub>	$\frac{1}{5}$	$\begin{array}{c} 23 \\ 56 \end{array}$	rhombic)Thallium aluminum sulfate dodecahydrate,	9	57
Silver bromate, AgBrO <sub>3</sub>	5	57	$TlAl(SO_4)_2 \cdot 12H_2O_1$	6	53
Silver bromide (bromyrite), AgBr Silver carbonate Ag <sub>2</sub> CO <sub>3</sub>	$^{ m 4}_{ m 1m}$	$\begin{array}{c} 46 \\ 44 \end{array}$	Thallium(I) arsenate, $Tl_3AsO_4$ Thallium(I) bromate, $TlBrO_3$	$\frac{2\mathrm{m}}{8}$	37 60
Silver chlorate, AgClO <sub>3</sub>	7	44	Thallium bromide, TlBr	7	57
Silver chloride (cerargyrite), AgCl	4	44	Thallium(I) chlorate, TlClO <sub>3</sub>	8	61
Silver iodide (iodyrite), AgI (hexagonal) Silver iodide, gamma, AgI (cubic)	8 9	51 48	Thallium (I) chloride, TlClThallium chloroplatinate, Tl <sub>2</sub> PtCl <sub>6</sub>	$\frac{4}{5}$	51 70
Silver metaperiodate, AgIO <sub>4</sub>	9	49	Thallium chlorostannate, Tl <sub>2</sub> SnCl <sub>6</sub>	6	54
Silver molybdate, Ag <sub>2</sub> MoO <sub>4</sub>	7 5	45 59	Thallium chromium sulfate dodccahydrate, TlCr(SO <sub>4</sub> ) <sub>2</sub> ·12H <sub>2</sub> O	6	55
Silver nitrite, $AgNO_2$	5	60	Thallium fluosilicate, $Tl_2SiF_{6}$	6	56
Silver oxide, $Ag_2O_{}$	1m	45	Thallium gallium sulfate dodecahydrate,	0	~=
Silver (II) oxynitrate, Ag <sub>7</sub> O <sub>8</sub> NO <sub>3</sub> Silver perrhenate, AgReO <sub>4</sub>	$\frac{4}{8}$	61 53	$TIGa(SO_4)_2 \cdot 12H_2O_{}$ Thallium(I) iodate, $TIIO_3_{}$	6 8	$\begin{array}{c} 57 \\ 62 \end{array}$
Silver phosphate, Ag <sub>3</sub> PO <sub>4</sub>	5	62	Thallium(I) iodide, TII, (orthorhombic)	4	53
Silver selenate, $Ag_2SeO_{4}$	2m	32	Thallium (I) nitrate, TlNO <sub>3</sub>	6	58
Silver sulfate, Ag <sub>2</sub> SO <sub>4</sub>	$\frac{7}{10}$	$\frac{46}{51}$	Thallium(III) oxidé, $Tl_2O_{3$	$^2_{ m 2m}$	$\frac{28}{38}$
Sodium acid fluoride, NaHF <sub>2</sub>	5	63	Thallium (I) phosphate, Tl <sub>3</sub> PO <sub>4</sub>	7	58
Sodium borohydride, NaBH <sub>4</sub>	9 5	51	Thallium (III) phosphate, TlPO	7	59 59
Sodium bromate, NaBrO <sub>3</sub> Sodium bromide, NaBr	$\frac{3}{3}$	$\begin{array}{c} 65 \\ 47 \end{array}$	Thallium(I) sulfate, Tl <sub>2</sub> SO <sub>4</sub> Thallium(I) thiocyanate, TlCNS	6 8	63
Sodium carbonate monohydrate (thermona-			Thallium(I) tungstate, Tl <sub>2</sub> WO <sub>4</sub>	1m	48
trite), $Na_2CO_3 \cdot H_2O$ Sodium chlorate, $NaClO_3$	$\frac{8}{3}$	$\frac{54}{51}$	Thorium oxide (thorianite), ThO <sub>2</sub>	$\frac{1}{9}$	57 58
Sodium chloride (halite), NaCl	$\frac{3}{2}$	41	Thulium sesquioxide, Tm <sub>2</sub> O <sub>3</sub> Tin, alpha, Sn (cubic)	$\frac{3}{2}$	12
Sodium cyanate, NaCNO	2m	33	Tin, beta, Sn (tetragonal)	1	$\frac{24}{2}$
Sodium cyanide, NaCN (cubic) Sodium cyanide, NaCN (orthorhombic)	$\frac{1}{1}$	$\begin{array}{c} 78 \\ 79 \end{array}$	$Tin(IV)$ iodide, $SnI_4$	5 4	$\begin{array}{c} 71 \\ 28 \end{array}$
Sodium fluoride (villiaumite), NaF	i	63	Tin(IV) oxide (cassiterite), SnO <sub>2</sub>	1	54
Sodium iodate, NaIO <sub>3</sub>	7	47	Tin(II) telluride, SnTe	7	61
Sodium iodide, NaISodium metaperiodate, NaIO <sub>4</sub>	$\frac{4}{7}$	31 48	Titanium, TiTitanium dioxide (anatase), TiO <sub>2</sub>	3 1	$\frac{1}{46}$
Sodium molybdate, Na <sub>2</sub> MoO <sub>4</sub>	$1 \mathrm{m}$	46	Titanium dioxide (rutile), TiO <sub>2</sub>	1	44
Sodium nitrate (soda-niter), NaNO <sub>3</sub>	6	50	Titanium(III) oxide, $TiO_{1\cdot\hat{a}15}$	9	59
Sodium nitrite, NaNO <sub>2</sub> ————————————————————————————————————	4	62	Titanium silicide, $Ti_5Si_3$ Tungsten, W	$\frac{8}{1}$	$\begin{array}{c} 64 \\ 28 \end{array}$
$Na_{2}WO_{4}\cdot 2H_{2}O_{$	$2 \mathrm{m}$	33	Tungsten sulfide (tungstenite), WS <sub>2</sub>	8	65
Sodium perchlorate, NaClO <sub>4</sub> (orthorhombic)	$\frac{7}{2}$	49	Uranium dioxide, $UO_{2$	$\frac{2}{7}$	$\begin{array}{c} 33 \\ 61 \end{array}$
Sodium sulfate (thenardite), Na <sub>2</sub> SO <sub>4</sub> Sodium sulfite, Na <sub>2</sub> SO <sub>3</sub>	$\frac{2}{3}$	59 60	Urea, $CO(NH_2)_2$	8	66
Sodium tetrametaphosphate tetrahydrate,			Ytterbium gallium oxide3:5, Yb <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>	$1 \mathrm{m}$	49
alpha, Na <sub>4</sub> P <sub>4</sub> O <sub>12</sub> ·4H <sub>2</sub> O (monoclinic) Sodium tetrametaphosphate tetrahydrate,	10	52	Yttrium arsenate, YAsO <sub>4</sub> Yttrium gallium oxide 3:5, Y <sub>3</sub> Ga <sub>2</sub> (GaO <sub>4</sub> ) <sub>3</sub>	$rac{2 ext{m}}{1 ext{m}}$	39 50
beta, Na <sub>4</sub> P <sub>4</sub> O <sub>12</sub> ·4H <sub>2</sub> O (triclinic)	2m	35	Yttrium, oxide, Y <sub>2</sub> O <sub>3</sub>	3	28
Sodium tungstate, Na <sub>2</sub> WO <sub>4</sub>	$1 \mathrm{m}$	47	Yttrium oxychloride, YOCl	1m	51
Strontium arsenate, Sr <sub>3</sub> (AsO <sub>4</sub> ) <sub>2</sub> Strontium bromide hexahydrate, SrBr <sub>2</sub> ·6H <sub>2</sub> O <sub>-</sub>	$rac{2 ext{m}}{4}$	36 60	Yttrium phosphate (xenotime), YPO <sub>4</sub>	8 1	$\begin{array}{c} 67 \\ 16 \end{array}$
Strontium carbonate (strontianite) SrCO <sub>3</sub>	$\hat{3}$	56	Zinc aluminate (gahnite), ZnAl <sub>2</sub> O <sub>4</sub>	$\frac{1}{2}$	38
Strontium chloride, SrCl <sub>2</sub>	4	40	Zine borate, ZnB <sub>2</sub> O <sub>4</sub>	$\frac{1}{2}$	83
Strontium chloride hexahydrate, SrCl <sub>2</sub> ·6H <sub>2</sub> O <sub>-</sub> Strontium fluoride, SrF <sub>2</sub>	$\frac{4}{5}$	58 67	Zinc carbonate (smithsonite), $ZnCO_{3}$ Zinc cyanide $Zn(CN)_{2}$	8 5	69 73
Strontium formate, $Sr(CHO_2)_{2-1-1-1}$	8	55	Zinc, fluoride, ZnF <sub>2</sub>	6	60
Strontium formate dihydrate, $Sr(CHO_2)_2$ .	0	56	Zinc fluosilicate hexahydrate, ZnSiF <sub>6</sub> ·6H <sub>2</sub> O <sub>2</sub> Zinc germanate, Zn <sub>2</sub> GeO <sub>4</sub>	8 10	70 56
2H <sub>2</sub> O orthorhombicStrontium iodide hexahydrate, SrI <sub>2</sub> ·6H <sub>2</sub> O	8 8	58	Zine germanate, $Zn_2GeO_4$ Zine iodide, $ZnI_2$	9	60
Strontium molybdate, SrMoO <sub>4</sub>	7	50	Zinc orthosilicate (willemite), Zn <sub>2</sub> SiO <sub>4</sub>	7	62
Strontium nitrate, $Sr(NO_3)_2$ Strontium oxide, $SrO_{}$	$\frac{1}{5}$	80 68	Zinc oxide (zincite), ZnOZinc pyrosilicate hydrate (hemimorphite)	2	25
Strontium peroxide, $SrO_2$	6	$\frac{52}{52}$	$Z_{n_4}(OH)_2Si_2O_7 \cdot H_2O_{}$	$\frac{2}{3}$	62
Strontium sulfate (celestite), SrSO <sub>4</sub>	$\frac{2}{2}$	61	Zinc selenide, ZnSe		23
Strontium sulfide, SrSStrontium titanate, SrTiO <sub>3</sub>	$\frac{7}{3}$	$\begin{array}{c} 52 \\ 44 \end{array}$	Zinc sulfate (zinkosite), ZnSO <sub>4</sub> Zinc sulfate heptahydrate (goslarite),	7	64
Strontium tungstate, SrWO <sub>4</sub>	7	53	ZnSO <sub>4</sub> ·7H <sub>2</sub> O	8	71
Strontium zirconate, SrZrO <sub>3</sub>	9	51	Zinc sulfide, alpha (wurtzite), ZnS	$\frac{2}{2}$	14
Sulfamic acid, NH <sub>3</sub> SO <sub>3</sub> Sulfur, S	9	$\begin{array}{c} 54 \\ 54 \end{array}$	Zinc sulfide, beta (sphalerite), ZnS Zinc tungstate, ZnWO <sub>4</sub>	$2 \mathrm{m}^2$	16 40
Tantalum, Ta	1	29	Zirconium, alpha, Zr	2	11
Tantalum Silicide, TaSi <sub>2</sub>	8 1	$\frac{59}{26}$	Zirconium iodate, Zr(IO <sub>3</sub> ) <sub>4</sub> Zirconium silicate (zircon), ZrSiO <sub>4</sub>	$\frac{1}{4}$	51 68
Tellurium, Te Tellurium(IV) oxide (paratellurite) TeO <sub>2</sub>	1	20	Zirconium sulfate tetrahydrate, Zr(SO <sub>4</sub> ) <sub>2</sub> .	_	
(tetragonal)	7	56	$4\mathrm{H}_2\mathrm{O}_{}$	7	66

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Andradite, Ca <sub>3</sub> Fe <sub>2</sub> Si <sub>3</sub> O <sub>12</sub>	9	$\frac{10}{22}$	Goslarite, ZnSO <sub>4</sub> ·7H <sub>2</sub> O <sub></sub>	8	71
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rhombic)	$1 \mathrm{m}$	28	Paratellurite, TeO <sub>2</sub>	7	56
Cordierite, Mg <sub>2</sub> Al <sub>4</sub> Si <sub>5</sub> O <sub>18</sub> ·(hexagonal)	1m	29	Partridgeite, Mn <sub>2</sub> O <sub>3</sub>	9	37
Corundum, Al <sub>2</sub> O <sub>3</sub>	9	3	Periclase, MgO	1	37
Cotunnite, PbCl <sub>2</sub>		45	Phenacite, Be <sub>2</sub> SiO <sub>4</sub>		11
Covellite, CuS	4	13	Picrochromite, MgCr <sub>2</sub> O <sub>4</sub>		34
Cristobalite, (alpha or low) SiO <sub>2</sub>			Portlandite, $Ca(OH)_2$		58
(Revised) Cristobalite, (beta or high) SiO <sub>2</sub>	10	<b>4</b> 8	Powellite, $CaMoO_{4}$		22
Cristobalite, (beta or high) SiO <sub>2</sub>	. 1	<b>4</b> 2	Pyrite, $FeS_{2}$	5	29
Cryptohalite, $(NH_4)_2SiF_{6}$	5	5	Quartz, SiO <sub>2</sub> (alpha or low)	3	24
Cuprite, $Cu_2O_{}$	2	23	Rammelsbergite, NiAs <sub>2</sub>	10	42
Diamond, C		5	Rhodochrosite, $MnCO_{3}$	7	32
Diaspore, $Al_2O_3 \cdot H_2O_{}$	3	41	Rutile, $TiO_2$	1	44
Enstatite, MgSiO <sub>3</sub>	6	32	Safflorite, CoFeAs <sub>4</sub>	10	28
Epsomite, MgSO <sub>4</sub> ·H <sub>2</sub> O <sub></sub>	7	30	Sal-ammoniac, NH <sub>4</sub> Cl	. 1	59
Ettringite, Al <sub>2</sub> O <sub>3</sub> ·6CaO·3SO <sub>3</sub> ·31H <sub>2</sub> O <sub>-</sub>	8	3	Scheelite, CaWO <sub>4</sub>		23
Fluorite, CaF <sub>2</sub>	1	69	Selenolite, SeO <sub>2</sub>	1	53
Forsterite, Mg <sub>2</sub> SiO <sub>4</sub>	1	83	Sellaite, $MgF_{2}$	4	33
Galaxite, MnAl <sub>2</sub> O <sub>4</sub>	. 9	35	Senarmontite, $Sb_2O_3$	3	31
Galena, PbS		18	Skutterudite, CoAs <sub>3</sub>	10	21

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Smithsonite, ZnCO <sub>3</sub>	_ 8	69	Tiemannite, HgSe		35
Soda-niter, NaNO <sub>3</sub>		50	Topaz, Al <sub>2</sub> SiO <sub>4</sub> (F,OH) <sub>2</sub>		4
Sphalerite, ZnS	_ 2	16	Trevorite, NiFe <sub>2</sub> O <sub>4</sub>		44
Spherocobaltite, CoCO <sub>3</sub>	_ 10	24	Tungstenite, WS <sub>2</sub>		$\overline{65}$
Spinel, MgAl <sub>2</sub> O <sub>4</sub>		35	Uvarovite, $Ca_3Cr_2(SiO_4)_3$		17
Stibnite, $Sb_2S_3$		6	Valentinite, Sb <sub>2</sub> O <sub>3</sub>		6
Stolzite, PbWO <sub>4</sub>		24	Villiaumite, NaF		63
Strontianite, SrCO <sub>3</sub>		56	Willemite, Zn <sub>2</sub> SiO <sub>4</sub>		62
Sylvite, KCl		65	Witherite, BaCO <sub>3</sub>		54
Tellurite, TeO <sub>2</sub> (orthorhombic)	_ 9	57	Wulfenite, PbMoO <sub>4</sub>		$\frac{1}{23}$
Tenorite, CuO		49	Wurtzite, ZnS		14
Teschemacherite, (NH <sub>4</sub> )HCO <sub>3</sub>		5	Xenotime, YPO <sub>4</sub>		67
Thenardite, Na <sub>2</sub> SO <sub>4</sub>		59	Zincite, ZnO		25
Thermonatrite, Na <sub>2</sub> CO <sub>3</sub> ·H <sub>2</sub> O <sub></sub>		54	Zinkosite, ZnSO <sub>4</sub>		$\overline{64}$
Thorianite, ThO <sub>2</sub>		57	$Zircon, ZrSiO_4$		68
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#### U.S. DEPARTMENT OF COMMERCE

Luther H. Hodges, Secretary

#### NATIONAL BUREAU OF STANDARDS

A. V. Astin, Director



### THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards at its major laboratories in Washington, D.C., and Boulder, Colorado, is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section carries out specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant publications, appears on the inside of the front cover.

#### WASHINGTON, D.C.

Electricity. Resistance and Reactance. Electrochemistry. Electrical Instruments. Magnetic Measurements. Dielectrics. High Voltage.

Metrology. Photometry and Colorimetry. Refractometry. Photographic Research. Length. Engineering Metrology. Mass and Scale. Volumetry and Densimetry.

Heat. Temperature Physics. Heat Measurements. Cryogenic Physics. Equation of State. Statistical Physics.

Radiation Physics. X-ray. Radioactivity. Radiation Theory. High Energy Radiation. Radiological Equipment. Nucleonic Instrumentation. Neutron Physics.

Analytical and Inorganic Chemistry. Pure Substances. Spectrochemistry. Solution Chemistry. Standard Reference Materials. Applied Analytical Research. Crystal Chemistry.

Mechanics. Sound. Pressure and Vacuum. Fluid Mechanics. Engineering Mechanics. Rheology. Combustion Controls.

Polymers. Macromolecules: Synthesis and Structure. Polymer Chemistry. Polymer Physics. Polymer Characterization. Polymer Evaluation and Testing. Applied Polymer Standards and Research. Dental Research.

Metallurgy. Engineering Metallurgy. Microscopy and Diffraction. Metal Reactions. Metal Physics. Electrolysis and Metal Deposition.

Inorganic Solids. Engineering Ceramics. Glass. Solid State Chemistry. Crystal Growth. Physical Properties. Crystallography.

Building Research. Structural Engineering. Fire Research. Mechanical Systems. Organic Building Materials. Codes and Safety Standards. Heat Transfer. Inorganic Building Materials. Metallic Building Materials.

Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Mathematical Physics. Opera-

tions Research.

Data Processing Systems. Components and Techniques. Computer Technology. Measurements Automation. Engineering Applications. Systems Analysis.

Atomic Physics. Spectroscopy. Infrared Spectroscopy. Far Ultraviolet Physics. Solid State Physics. Electron Physics. Atomic Physics. Plasma Spectroscopy.

Instrumentation. Engineering Electronics. Electron Devices. Electronic Instrumentation. Mechanical Instruments. Basic Instrumentation.

Physical Chemistry. Thermochemistry. Surface Chemistry. Organic Chemistry. Molecular Spectroscopy. Elementary Processes. Mass Spectrometry. Photochemistry and Radiation Chemistry.

Office of Weights and Measures.

## BOULDER, COLO.

Cryogenic Engineering Laboratory. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Cryogenic Technical Services.

#### CENTRAL RADIO PROPAGATION LABORATORY

Ionosphere Research and Propagation. Low Frequency and Very Low Frequency Research. Ionosphere Research. Prediction Services. Sun-Earth Relationships. Field Engineering. Radio Warning Services. Vertical Soundings

Radio Propagation Engineering. Data Reduction Instrumentation. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Propagation-Terrain Effects. Radio-Meteorology. Lower Atmosphere Physics.

Radio Systems. Applied Electromagnetic Theory. High Frequency and Very High Frequency Research. Frequency Utilization. Modulation Research. Antenna Research. Radiodetermination.

Upper Atmosphere and Space Physics. Upper Atmosphere and Plasma Physics. High Latitude Ionosphere Physics. Ionosphere and Exosphere Scatter. Airglow and Aurora. Ionospheric Radio Astronomy.

#### RADIO STANDARDS LABORATORY

Radio Physics. Radio Broadcast Service. Radio and Microwave Materials. Atomic Frequency and Time-Interval Standards. Radio Plasma. Millimeter-Wave Research.

Circuit Standards. High Frequency Electrical Standards. High Frequency Calibration Services. High Frequency Impedance Standards. Microwave Calibration Services. Microwave Circuit Standards. Low Frequency Calibration Services.

